Performance Assessment of Plant Extracts as Green Demulsifiers

by

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13938

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
Petroleum Engineering Programme
Universiti Teknologi PETRONAS
in partial fulfillment of the requirement for the
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Approved by,

_____

(Dr Aliyu Adebayor Sulaimon)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
May 2014

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

YAAKOB BIN ABU BAKAR

ABSTRACT

This project is about the demulsifier formulation by using plant extract to produce a green demulsifier. Demulsifier is an oilfield chemical that is used to be injected into Water-in-Oil (W/O) emulsion to be separated into water and oil. Current conventional demulsifiers that available in markets are likely to give bad impacts towards the environment due to high toxic level. The objective of this project is to study and select the most suitable plants that have high potential to be used as green demulsifier. This project is also to observe, evaluate and develop the performances assessment of the plant extracts towards the synthetic emulsion crude sample.

The plants that used are green tea, olive and coconut because of the fatty acid, naphthenic acid and polyphenols content. There are five main processes involved in this project which are samples preparation that used Soxhlet Extraction method to extract the plants, identification of the plant extract's compositions using Gas Chromatography Mass Spectrometer (GC-MS), static and dynamic bottle test, toxicity level test and performance assessment development. In order to provide the significant impact of the plant extracts and also as the comparison purpose, the author also formulated blend demulsifier from local materials such as starch, camphor, Calcium Hydroxide $Ca(OH)_2$, Sodium Hydroxide NaOH, paraffix wax, liquid soap and distilled water.

Based on the results obtained from both static and dynamic test, there are six best formulations that give good results from all 23 of formulations which are SR1637, B2, E2 and E3 which are olive and coconut extract, FE2 and FI1. SR1637 is the industry chemical that currently used, B2 is a blend demusifier that consists of NaOH, E3 extract and other materials like starch, camphor, paraffin wax, liquid soap and distilled water, FE2 is a combination of two best plant extracts which are E2 and E3 and FI1 is the combination between E3 and SR1637. In terms of toxicity level, B2 is the most toxic demulsifier as the pH value is 12 means that it has alkali property and E3 contain the least toxic level as the pH value is 6 that is a neutral demulsifier. From all of these six formulations, E3 extract give the best performances in separation process of W/O emulsion.

As the conclusion, E3 extract selected to be the most effective green demulsiifer with low toxicity level and able to separate water of about 90 % to 95%. Demulsifier is very important in oil and gas industry as it is widely used in production phase of oil in order to optimize the oil production. This green demulsifier is also very benefit to the environment as it is contain 100% of organic materials which is coconut and could reduce the harmful effects towards the environment. The cost of producing this green demulsifier also low as it is locally available in South East Asia especially Malaysia and this plant also easy to obtained.

ACKNOWLEDEMENT

I would like to express my gratitude and great appreciation to those who help me a lot in completing this report. A special thanks to my Supervisor, Dr. Aliyu Adebayor Sulaimon, Senior Lecturer of Department of Petroleum Engineering, who have given his full effort in guiding me in achieving the goal as well as his encouragement to keep up my motivation and performances in completing this Final Year Project.

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NOMENCLATURE

E	Plant extract
B	Blend demulsifier
FE	Formulation for combination of E2 and E3
FI	Formulation for combination of E3 and SR 1637
Ca(OH)2	Calcium Hydroxide
NaOH	Sodium Hydroxide

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Oil is produced from the reservoirs in association with the natural formation water and could probably mix together with the presence of sufficient agitation to form an emulsion. Formation of the emulsion has a very significant effect to the production facilities at the surface and the amount of oil recovery and is undesirable. There are several techniques must be carried out to break the emulsion, whether by the application of heat, mechanical or chemical (Kamaruddin, 2010) [1]. All the techniques to break the emulsion are called as demulsification process. In this project, the author will focus on the chemical part of demulsification with the project title is "Performance Assessment of Plant Extracts as Green Demulsifier".

The emulsion is likely to form when there are two immiscible liquids mixed together, which is one are dispersed as droplets in the other (Fingas, 2014) [2]. The size of the droplets can be of all ranges in size, from large size that are visible to sub micron in size. Most of emulsions are thermodynamically unstable. There are possibility and tendency for the system and other mechanisms to reduce the interfacial energy and separate the water and oil emulsion.

Demulsifiers are normally polymeric surfactants such as copolymers of polyoxyethelene and polypropylene, alkylphenol-formaldehyde resins or blends of various surface active substances (Dalmazzone & Noik, 2001) [3]. All these kind of demulsifier have been used widely in current industries. Due to the concern towards the environment, the safer formulation, less toxic, but as efficient as the conventional demulsifier need to be formulated and used instead of the conventional demulsifier. The less toxic demulsifier can be termed as "Green Demulsifier".

Based on the project title, the author must conduct several experiments in order to develop the performance assessment. There are four major processes that involve in this project, which are samples preparation that are plant extract samples and synthetic

emulsion crude samples. The second process is identifying the presenting of hexane group, including methyl-cyclohexane, nitrocyclohexane and cyclohexanecarboxylic acid and also Octadecenoic acid in the plant extracts. The next stage is conducting bottle test by using synthetic emulsion crude that is heated at 60℃ to assist the breaking process of the emulsion and lastly is the performance evaluation development by using the results that obtained from the bottle test by observing the amount and quality of water separated, time separation between water and oil with respect to the amount of plant extract used.

Prior to conducting the experiment, the author needs to study about the plants that have high potential to be used in this project. Analysis of the compositions of the plants is necessary to ensure the performance effectiveness and to minimize the harmful effects towards the environment by considering the pH value of that chemical. A chemical that has acidic property or with low pH value as well a chemical that has alkaline property or with high pH value tend to contain highly toxic (Sharon) [4]. There are three types of plants that have been found to have high potential to be used in this project that are green tea leaves, olive and coconut. All these plants are readily available in Malaysia. In order to provide the significant impact of the plant extracts and also as the comparison towards the emulsion breaking process, the author also formulated blend demulsifier from local materials such as starch, camphor, $Ca(OH)_2$, NaOH, paraffix wax, liquid soap and distilled water.

1.2 Problem Statement

Commercial and conventional demulsifiers that are available in markets proved to give good results and effective in separating water in oil emulsion that form in oil and gas industry. This conventional demusifier commonly polymeric surfactants such as polypropylene, polyoxyethelene and contains methyl benzene. All these compounds are harmful when exposed to the environment. Demulsifier is injected at the point of injection causing water and oil to be separated. The separated water will undergo further treatment before it is discharged to the sea. Sea water and the aquatic marine life is exposed to all these chemical substances directly that contain in the water.

Land, groundwater and air also can be contaminated by this chemical exposure, which is normally caused by chemical spillage that is likely to occur during manufacturing, packing, delivering and transferring process. As a conclusion, the main concern that leads to this project is the environmental issue. The bad impacts towards the environment can be reduced by the formulation of synthetic demulsifier that can be termed as "Green Demulsifier". This "Green Demulsifier" is formulated from the extraction of plants as well as blend demulsifier that consists of the materials that is easy to get and available in Malaysia. The result of this experiment is compared with the conventional demulsifier that currently used in the industry for the performance comparison.

1.3 Objectives of the Study

The objectives of this project are to study the potential of the plants to be used as green demulsifiers by extraction process and the potential of those plants to be used in real situations as an alternative to the conventional demulsifier by taking account the environmental issue. This project also carried out to observe, evaluate and develop the performances of the plant extracts towards the synthetic emulsion crude sample. Finally, this project is aimed to determine the most effective "Green Demulsifier" based on the certain criteria which are the volume of water separated from the crude oil and the time for water to be separated from crude oil by considering the amount of the demulsifier used.

1.4 Scopes of the Study

This project requires the author to study and understand the concept of emulsion which is focused on the water in oil emulsion including the demulsification process. Prior to the experiment in the laboratory, the author is conducted studies and selected three types of plants that have high potential to be used as "Green Demulsifier" that, green tea leave olive and coconut. The extraction process has taken place in the laboratory to get the plant extracts by using a Soxhlet extraction method as well as synthetic water in oil emulsion creation. The author also is developing the performance assessment by testing the plant extracts and blend demulsifier that consists of local raw materials. Static and

dynamic bottle test is conducted in the laboratory by using water bath and also bench centrifuge.

1.5 Relevancy and Feasibility

This project is relevant to the program studied as this project is strongly related with oil and gas industry. Demulsifier is one of the important chemicals as it is able to define and optimized the amount of oil reserves. This project mainly focused on the green demulsifier development and very related with the global current issue in oil and gas industry and also other industry as an effort for the environment conservation.

The plants selected used in this project are relevant as that plants are containing fatty acid, naphthenic acid and also polyphenols that can react as the surfactant and reducing the interfacial tension energy. Eventually the film that surrounding the water droplets is broken and separate the emulsion into water and oil.

The equipments chosen in this project also relevant and available in the laboratory such as Soxhlet extractor used to extract the plants, rotary evaporator to separate the plant extracts from the solvent and bench centrifuge used to run the test in dynamic condition.

In terms of the feasibility of the project, the allocated period is about 28 weeks that are within two semesters. Students need to accomplish the project assigned within this period. Regarding with this project, the author found that this project is feasible to complete within the allocated time and job scopes studied.

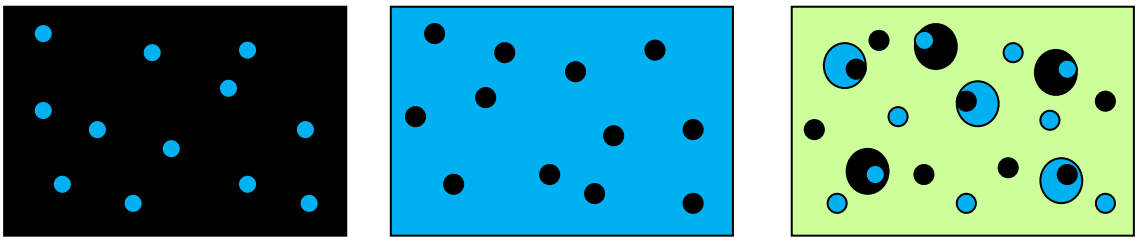
CHAPTER 2

LITERATURE REVIEW

2.1 Emulsion

An emulsion is a mixture of two immiscible liquids whereby one is dispersed as droplets in the other. This type of liquid is known as the internal phase, the liquid that surrounds the droplets is called as external phase or continuous phase. Emulsion can be divided into three types, water in oil (W/O) emulsion, oil in water (O/W) emulsion and multiphase emulsion (Lowe, 1937) [5]. The first type of emulsions that is water-in-oil (W/O) emulsion where water is the dispersed phase and oil is the continuous phase. This type of emulsion often occurred during the production of oil and water. Dehydration method can be used in order to treat this kind of emulsion.

Second type of emulsion is oil-in-water (O/W) emulsion which is oil is the dispersed phase and water is the continuous phase. This type of emulsion can be encountered in the water that has been separated from the dehydration process. The De - oiling method can be used in order to treat this type of emulsion. The last type of emulsion is a multi phase emulsion which consists both water in oil emulsion and oil in water emulsion simultaneously. This type of emulsion is often occurred in slope of oil systems and storage tanks.



a) Water-in-Oil Emulsion b) Oil-in-Water Emulsion c) Multiphase Emulsion

Figure 2.1 Types of emulsion

Considering this phenomenon, emulsions that formed in the petroleum industry are predominantly water in oil (W/O) emulsion (Syauqi, 2009) [6]. Emulsions of oil and water are one of many problems occurred that directly associated with the petroleum

industry, both in oil field production and refinery stage. There are three main conditions that encourage the stability of the emulsion, whereby the liquids involved must be immiscible, the presence of the emulsifying agent or emulsifier and a sufficient agitation is needed to make one liquid is dispersed as droplets in another.

Emulsions are made up of two or more liquids that will not mix naturally and emulsifying agent is needed. In the petroleum industry, the most common emulsifying agents found include asphaltenes, solid paraffins, resinous substances, naphthenic and other oil soluble organic acids and materials that are soluble, dispersal and wet table in oil than water . Materials like zinc, iron, aluminium sulfates, calcium carbonates, silica and iron sulfade also found in the emulsions which are often found at the interface between the oil and droplets of water in the form of a film around the droplets.

The flowing wells that produced through chokes, gas lift and air lift can cause emulsion problems. The methods of production also contribute to the formation of emulsions. Mayonnaise, ice cream, soap and body lotion are the examples of stable emulsions (Kokal, 2002) [7]. There are four main factors that affect the stability of the emulsion that are viscosity, specific gravity, water percentage and age of emulsion.

Viscosity of liquids often defined as the resistance to flow. As the viscosity of the liquid is getting higher, the resistance of the liquid to flow also is greater and vice versa. Often, if a liquid of high viscosity is being heated, the viscosity of the liquid tends to decrease and causes the liquid to flow more freely. Oil with high viscosity needs more time for the water droplets to coalesce and settle out than the oil with low viscosity. Specific gravity and API gravity are two different parameters as the specific gravity of a liquid substance is the weight of a given amount of that liquid at a given temperature compared to the weight of an equal volume of water at the same temperature. The relationship between specific gravity and API gravity can be illustrated by using the formula below.

$$\text{API Gravity} = \frac{141.5}{\text{Specific Gravity}} - 131.5 \qquad \ldots \qquad (2.1)$$

Heavy oil with a high specific gravity and low API gravity in water in oil emulsion tends to cause the water droplets in suspension longer than the oil with low specific gravity and high API gravity.

Water percentage can be defined as the relative proportion of oil and water produced. A small percentage of water that contains in oil will emulsify more thoroughly and permanently than a large water percentage. The wells that producing only small quantities of water will form a tight emulsion and this emulsion will almost completely disappear if the percentage of water is increased beyond a certain limit.

The crude oil emulsions are the systems that are not in stable equilibrium. Based on the laws of thermodynamics, this type of systems will change continually in order to attain equilibrium. As a result, the stability of the emulsions will increase with age and the resistance to dehydration also increased.

2.2 Theories of Demulsification

Demulsification is a process of breaking down the emulsion problems through some treating methods into water and oil. There are many theories regarding the problem of resolving crude oil emulsions such as reverse phase, rigid film, pH, electronic charge, temperature and surface tension.

In the rigid film theory, the present of the reagents is to assist in the emulsion breaking process by converting the film from a plastic or can be assumed as distensible envelope to a glass like which has a relatively low coefficient of expansion. As the enclosed water is undergoing the heating process and expand to be shattered and finally the emulsion is broken. Emulsion also can be broken down through neutralization by changing in pH or loss of solubility. The efficiency of demulsification is attained at a neutral pH (Azim, et al., 2010) [8]. Emulsifying agents are polar bodies which have negative or positive charges to function and therefore any bodies that present with opposite charges should encourage the emulsion to break.

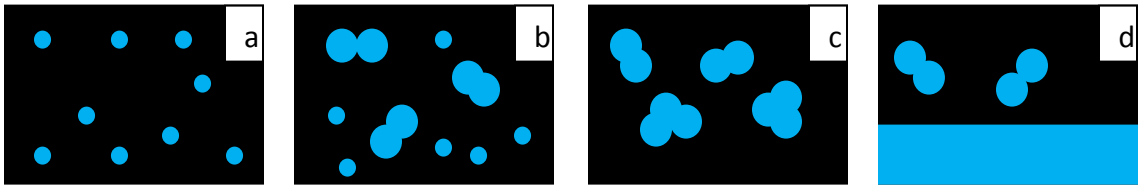
Sufficient heat is needed for the state of the film to change. As the film experience an increasing heat, the particles that form the film will collide each other and finally the

bonding between the particles will break for the emulsion to break. Based on this theory, the interface between the dispersed phase and the continuous phase is modified in some manner. The liquid that having the greater surface tension will act as the dispersed phase and the liquid that having the lower surface tension will act as the continuous phase.

2.3 Plants Selected

In this project, plant extracts are used in order to formulate the green demulsifier and this plant extraction is tested on the synthetic emulsion crude sample. There are two main plant compositions that are able to break the emulsion by specific approaches that are hexane group and Octadecenoic acid. Both of these compositions can be found in plants like green tea, olive, coconut and most grains. In this project the author will use three types of plants that are green tea leaves, olive and coconut.

These compositions extracted from all of the plants will react as the demulsifier that must have surfactant behavior that are able to flocculate the water droplets, able to coalesce the water droplets and wet ability of solids (Chester & David, 1996) [9]. In the process of breaking the emulsion, there are four stages that involved which are water present as small droplets in the oil, flocculation of the water droplets, coalescence of the water droplets and finally is the settling down of larger droplets.



a) Water Present as Small Droplets in Oil
b) Flocculation of the Water Droplets
c) Coalescence of the Water Droplets
d) Settling Down of Larger Droplets

Figure 2.2 Steps of water-in-Oil emulsion breaking process

In the early stage, the water in oil is present as the small droplets. Once the demulsifier is injected into the water in oil emulsion, the demulsifier will travel through the oil to reach the water droplets. The emulsifying agent is then displaced by the demulsifier as the surface active character. Ultimately the surface tension and interfacial energy of the water droplets is lowered. The water droplets then will move toward each other and form

flocculation as the surface of the droplets has an affinity to each other. The large water droplets resulted from the flocculation process then are coalesced to form larger droplets once the droplets are close together. Considering the effect of gravitational energy, the coalesced droplets move downwards through the oil and finally settled out at the bottom of the treating vessel as the droplets become heavier.

2.4 Blend Demulsifier Materials

Blend demulsifiers are being used in this project to be tested with the synthetic emulsion crude sample in order to develop the performance assessment and compare the results with the plant extracts as well as mix the plant extract with this type of demulsifier if necessary. The materials that used to formulate these blend demulsifiers are tapioca starch, camphor, $Ca(OH)_2$, NaOH, paraffin wax, liquid soap and distilled water. Each of these materials has specific functions that can cause the water-in-oil emulsion to be separated. In fact, the formulation of blend demulsifier able to neutralize the stabilizing effect of emulsifying agents that present in the emulsion crude sample (Emuchay, et al., 2013) [10]. The table below shows the local materials which are from various sources with the specific functions.

Table 2.1 Local materials with specific functions

No.	Materials	Function
1	Starch	As a water repellant
2	Camphor	As a solid wetting and viscosity adjuster
3	$Ca(OH)_2$/ NaOH	As a flocculants
4	Paraffin wax	As a water repellent
5	Liquid soap	As a surfactant that gives good interface
6	Distilled water	As a solvent

Chemically, both NaOH and $Ca(OH)_2$ have some important differences. $Ca(OH)_2$ or also called as slaked lime is a white powder that has two hydroxyl groups (Barekatain, Hasheminia, & Attary, 2012) [11]. Meanwhile, NaOH is a colorless crystal that has one hydroxyl group. Due to this difference in structural formula, both of these chemicals are

being mixed in two different formulations in order to observe which one is the best flocculant although both are good in the flocculation process (Morgan, 2011) [12].

CHAPTER 3

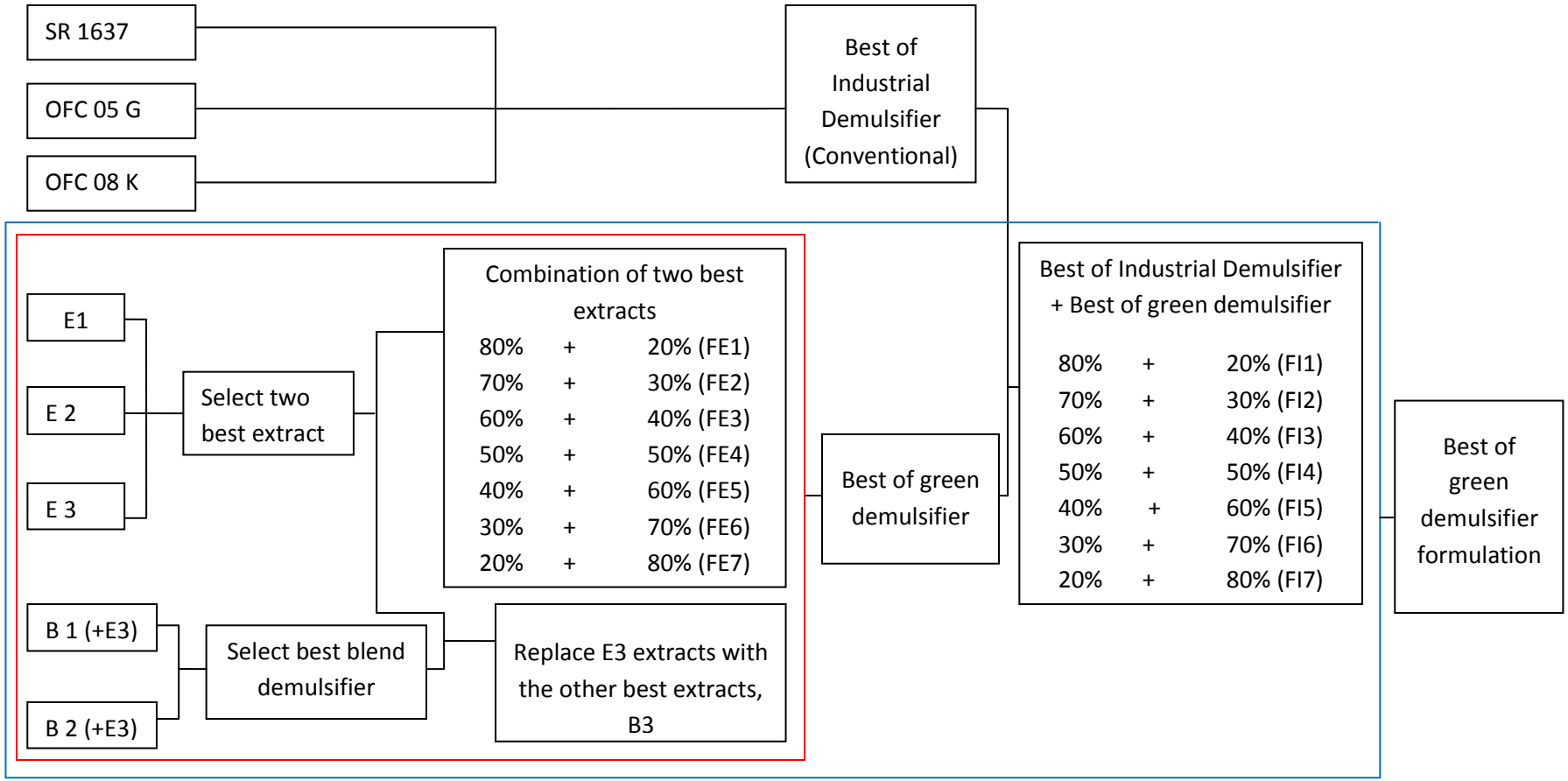
METHODOLOGY / PROJECT WORK

3.1 Methodology

In order to complete this project, there are five main processes involved which are samples preparation, plant extracts compositions identification, static and dynamic bottle test, toxicity level test and performance assessment development.

In samples preparation process, there are three types of samples is prepared which are plant extracts by using soxhlet extractor, blend demulsifier samples and also synthetic water-in-oil emulsion. The compositions of the plant extracts is identified by using Gas Chromatography Mass Spectrometer (GC-MS) and for this purpose, the samples are sent to the central laboratory. In experimentation process, all of the formulations is tested both in static and dynamic condition. All the formulations is divided into five main groups which are conventional demulsifier, plant extracts, blend demulsifier, combination between two best plant extracts and also combination between the best plant extracts and the best conventional demulsifier.

In order to identify the toxicity level of the formulations, there are two tests carried out which are aquatic toxicology test and also pH value test. Finally is the performance assessment development process. At this stage, there are four main criterias that considered such as the volume of water separated, the time taken for water and oil separated, quality of water separated and the amount of the demulsifier used.



E1 = Green tea extract
E2 = Olive extract
E3 = Coconut extract

B1 = Blend demulsifier using $Ca(OH)_2$
B2 = Blend demulsifier using NaOH

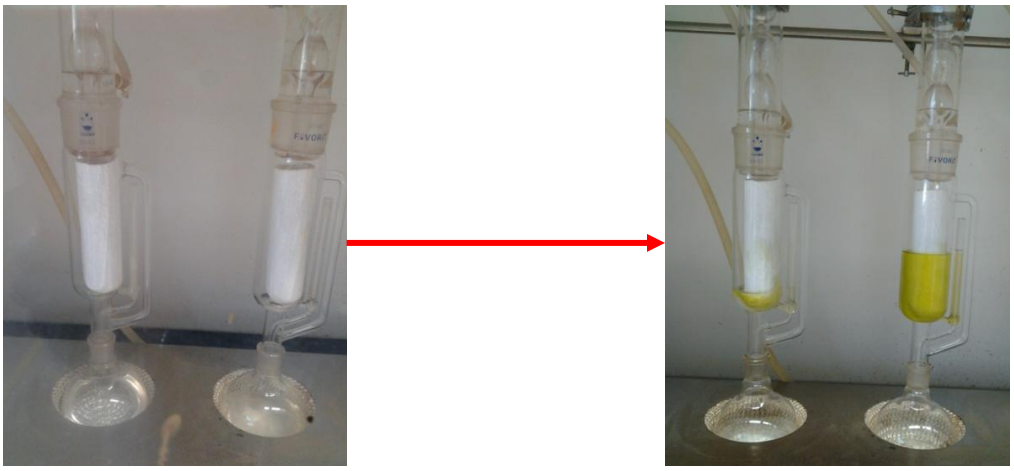
Figure 3.1 Flow chart for experiment design

3.2 Project Activities

This project involves some processes that must be carried out such as plant extraction process, identification of plant extracts compositions, preparation of the blend demulsifier sample, preparation of synthetic emulsion crude sample, static bottle test, dynamic bottle test and performance evaluation.

3.2.1 Plant Extraction Process

In this process, the plant leaves are dried in the oven for about 12 hours, while the temperature is maintained at 60℃. The leaves are ground until become powder by using mortal grinder.The plant powder is extracted by using Soxhlet extraction where the plant powder is located in the Soxhlet Thimble and ethanol is used as the solvent that placed in the round bottom flask. The estimated amount of ethanol that is used is 6ml for 1g of plants. The extraction process would take around 24 hours. The plant extractions then separated from ethanol by using a rotary evaporator with the parameters used are 100rpm at 60℃-70℃. This separation process would take about 30 minutes. The plant extraction undergone composition identification using Gas Chromatography Mass Spectrometer (GCMS). The plant extracts are named as E1 for green tea extract, E2 for olive extract and E3 for coconut extract.



a) Plant extraction before one cycle b) Plant extraction after one cycle

Figure 3.2 Plant extraction process by using soxhlet extractor

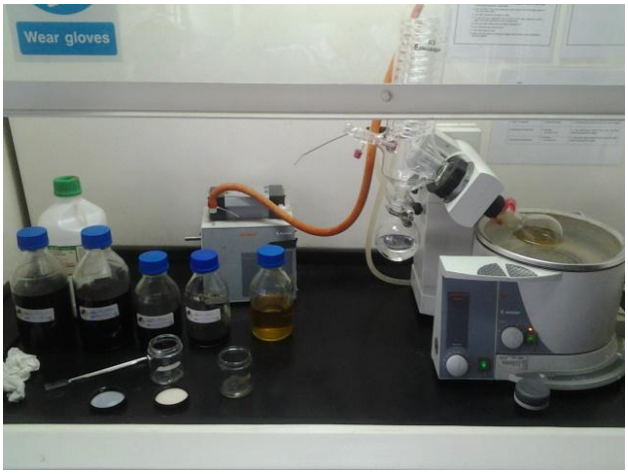


Figure 3.3 Separation of plant extracts from the extraction solvent (ethanol) by using a rotary evaporator

3.2.2 Identification of Plant Extracts Compositions

Identification of plant extract compositions is made by using Gas Chromatography-Mass Spectrometer. In this gas chromatography analysis, the temperature of the oven is maintained at 100℃ for 5 minutes. The temperature is increased up to 375℃ at a rate of 20℃/min and is maintained for 5 minutes. The injector temperature is about 350℃ and the transfer line temperature is about 300℃. For this test, the plant extract samples are sent to the block P.

3.2.3 Preparation of Blend Demulsifier Sample

Two different blend demulsifier formulations that consist of seven local materials whereby each having its own specific functions is prepared. First formulation of blend demulsifier is consists of E3, starch, camphor, flocculants Ca(OH)2, paraffin wax , liquid soap and distilled water that is formulated in percentage basis and named as B1. Another blend is formulated by using NaOH instead of Ca(OH)2 and named as B2. The main objective of this blend demulsifier samples preparation is to determine the effect of adding Ca(OH)2 and NaOH towards the parameters measured since both are good as flocculent but with different hydroxyl group number. Besides, the other objective is to

determine the effect of E3 towards the parameters measured since E3 extract is the best dehydrating agent compared with the other two extracts.

These two formulations is tested with the synthetic emulsion crude samples. Formulation that gives good results will further formulated by replacing the E3 extract with the other two plant extracts that will give the best result either E1 or E2 extract. For example, if sample B1 shows good result, sample B2 is ignored and the sample for B1 is further formulated by replacing the E3 extract with the plant extract that will give the best result that is either E1 or E2 extract. The formulation for blend demulsifier samples is provided in the APPENDIX II.

3.2.4 Preparation of Synthetic Water-in-Oil Emulsion Sample

Synthetic water in oil emulsion crude sample is prepared to be used for the testing purposes. The testing is conducted by adding the formulated demulsifiers. There are two main materials that is used to prepare this sample which are crude oil and brine water of 90,000 ppm.This synthetic water in oil emulsion has been formulated by mixing 50% crude oil and 50% brine water. The mixture is then being stirred for about 20 minutes in order to make it well mixed. The emulsion is filled in the centrifuge tube for about 25ml for testing purpose.

Figure 3.4 Preparation of synthetic emulsion crude sample

3.2.5 Static Bottle Test

Static bottle test is carried out to get the results for the emulsion breaking process in the static condition. Before the test begins, the synthetic emulsion crude sample is placed in the water bath first at 60℃ for 10 minutes in order to assist the separation of the emulsion and also to simulate it with the actual condition temperature. In this test, 0.5 ml of demulsifier sample is injected into 25 ml of emulsion samples and labels it with the name of the demulsifier injected.

The centrifuge tube is closed and is shaken manually for 100 times continuously. After shaking, the sample is kept in the water bath again. The amount of water and oil separated is measured at 10 minutes, 30 minutes, 60 minutes and 120 minutes. The results obtained are recorded on the result sheet. The experiment is repeated with 1.0 ml and 1.5 ml amount of demulsifier used and also tested with different type of demulsifiers.

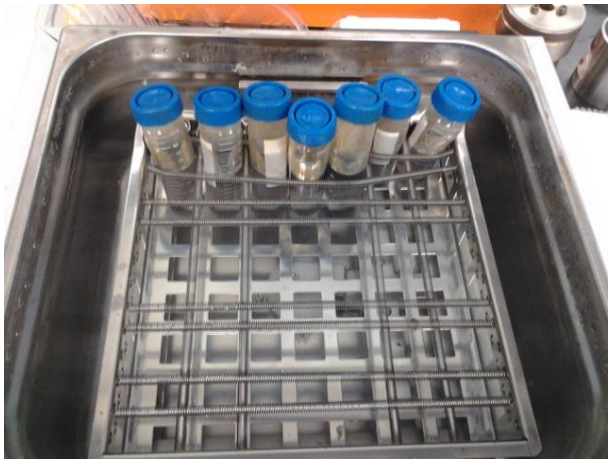


Figure 3.5 Static bottle test

3.2.6 Dynamic Bottle Test

Generally, the process for the dynamic bottle test is almost the same with the static bottle test which is carried out to get the results for the emulsion breaking process but in dynamic condition. In this test, 0.5 ml of demulsifier sample is added into the centrifuge tube that contain the synthetic emulsion crude sample of 25 ml and the centrifuge tube is immersed in the water bath for 10 minutes at the operating temperature that is 60℃. The

injected sample is put in the bench centrifuge and spun for 10 minutes at 2000rpm. The column separation of water from the crude is read and recorded immediately after the bench centrifuge is stopped. The experiment is repeated with 1.0 ml and 1.5 ml of demulsifier amount and also tested with different type of demulsifier.

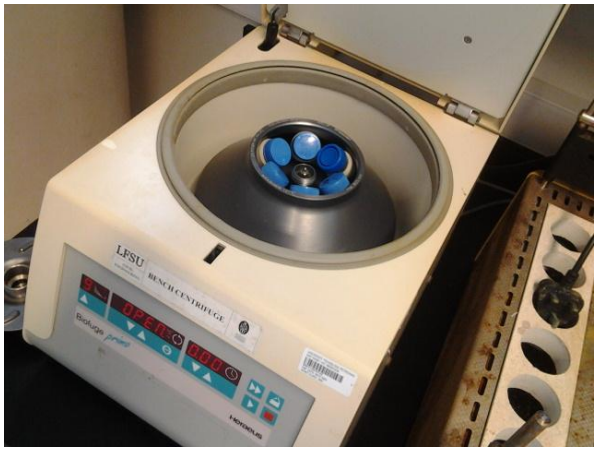


Figure 3.6 Dynamic bottle test by using a bench centrifuge

3.2.7 Toxicity Level Test

Since the objective of this project is to come out with a green demulsifier formulation, the measuring process of the toxicity level of the demulsifiers formulated is necessary. In this part, the author have used two techniques which are using fish or known as Aquatic Toxicology Tests and the pH value test.

Aquatic Toxicology Test is carried out by filling a container with 100 ml of tap water and is injected with 0.5 ml of the demulsifiers formulated. A fish is placed in that container and the time taken for the fish to die is recorded in minutes. pH value test is carried out as a confirmation test for the previous test, Aquatic Toxicology Test. This test is done by immersed the pH paper into the water that already injected with the demulsifiers. The value of the pH test is recorded.

Figure 3.7 Aquatic toxicology test

3.2.8 Performance Evaluation

This project requires the author to develop the performance assessment and evaluation of the testing conducted. There are four main parameters observed and evaluated at this stage such as the amount of the water separated, the quality of the water separated, the separation time between water and oil and the amount of extracts used. All these parameters also depend on the test condition either static or dynamic.

Table 3.1 Example of result sheet for static bottle test

No.	Product	Demulsifier dosage (ml)	Volume separation of water (ml) with time (min)					Water quality after 120 min
			0 min	10 min	30 min	60 min	120 min	
1								
2								
3								

Table 3.2 Example of result sheet for dynamic bottle test

No	Products	Demulsifier dosage, ml			Water quality
		0.5	1.0	1.5	
1					
2					
3					

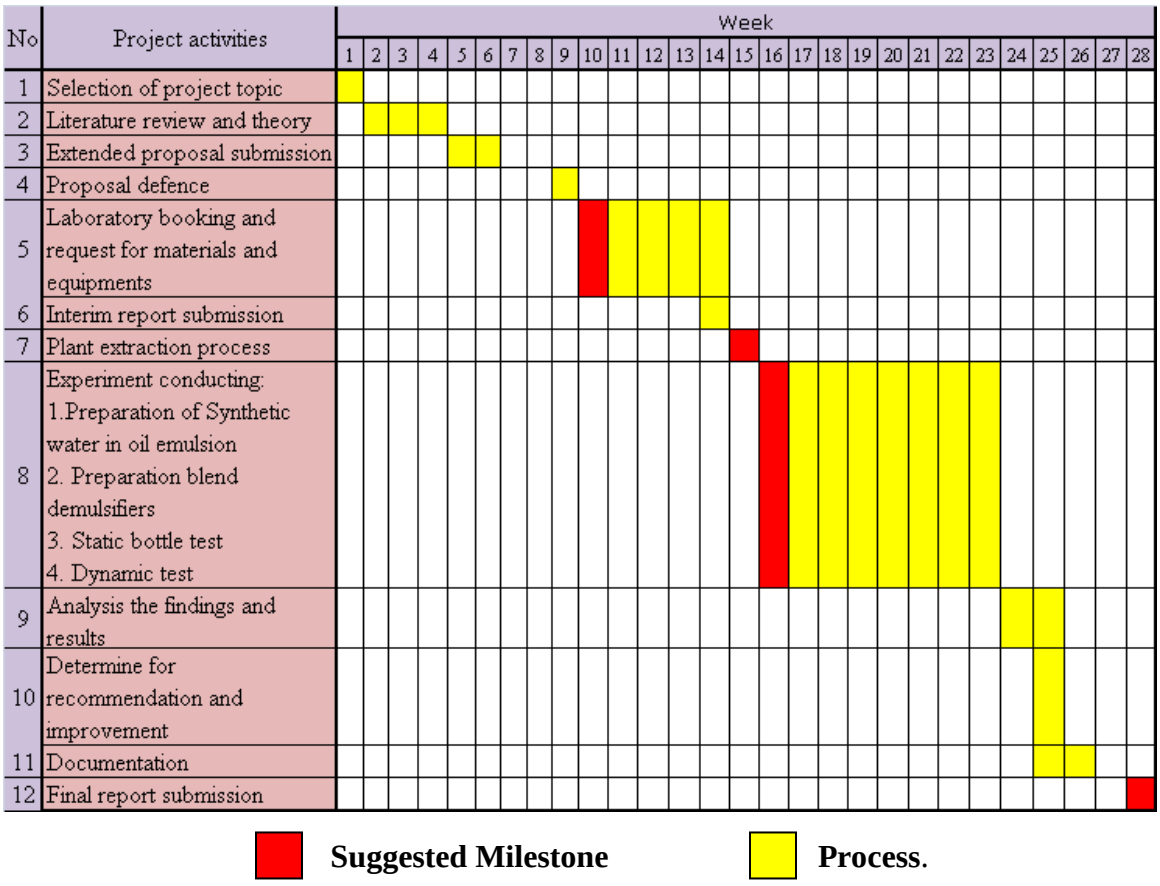
3.3 Key Project Milestone

Table 3.3 Key project milestone

Suggested Milestone	Week
Early research development: Involve research background, scope of studies and assumptions, information gathering and identify the tools and materials needed	1-9
Middle research development: Involve development of the procedure, requesting for materials and equipments and conducting the experiment.	10-23
Final research: Involve the analyzing process of the results obtained from the experiment, finalizing the result and completing the documentation.	24-26

3.4 Project Timeline (Gantt Chart)

Table 3.4 Project timeline (Gantt Chart)



3.5 Tools and Materials

Table 3.5 shows the main tools that are required for the experiment conducting for this project.

Table 3.5 Main tools required for experiment

No	Tools
1	Soxhlet thimble, water bath, oven
2	Mortal grinder
3	Rotary evaporator,
4	Bench centrifuge
5	Gas Chromatography-Mass Spectrometer (GCMS)

Table 3.6 shows the main materials that are required to carry out the testing.

Table 3.6 Main materials required to carry out the testing

No.	Materials
1	Crude oil
2	Brine water, 0.9%
3	Coconut extract
4	Starch
5	Camphor
6	Green tea
7	$Ca(OH)_2$
8	NaOH
9	Paraffin wax
10	Distilled water
11	Ethanol
12	Olive extract

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Static Bottle Test

The results that obtained are recorded on the result sheet. The author has divided the test into six parts that are static bottle test for conventional demulsifiers, static test for plant extracts, static test for blend demulsifiers, static test for blend demulsifier by replacing the E3 extract with the best plant extract, static test for combination of E3 and the best plant extract as well as static test for combination of the best conventional demulsifier with the best green demulsifier formulations. Tables below show the results obtained.

Table 4.1 Results for static bottle test of conventional demulsifier

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	SR 1637	0.5	0	9	11	12	12.5	Clear
		1.0	0	9	12	12	12.5	Clear
		1.5	0	10	10	11	12	Clear
2	OFC 05 G	0.5	0	1	5	7	9	Hazy
		1.0	0	3	5	9	9	Hazy
		1.5	0	3	7	9	10	Slighly hazy
3	OFC 08 K	0.5	0	3	3	5	7	Hazy
		1.0	0	3	3	6	9	Hazy
		1.5	0	5	7	7	10	Hazy

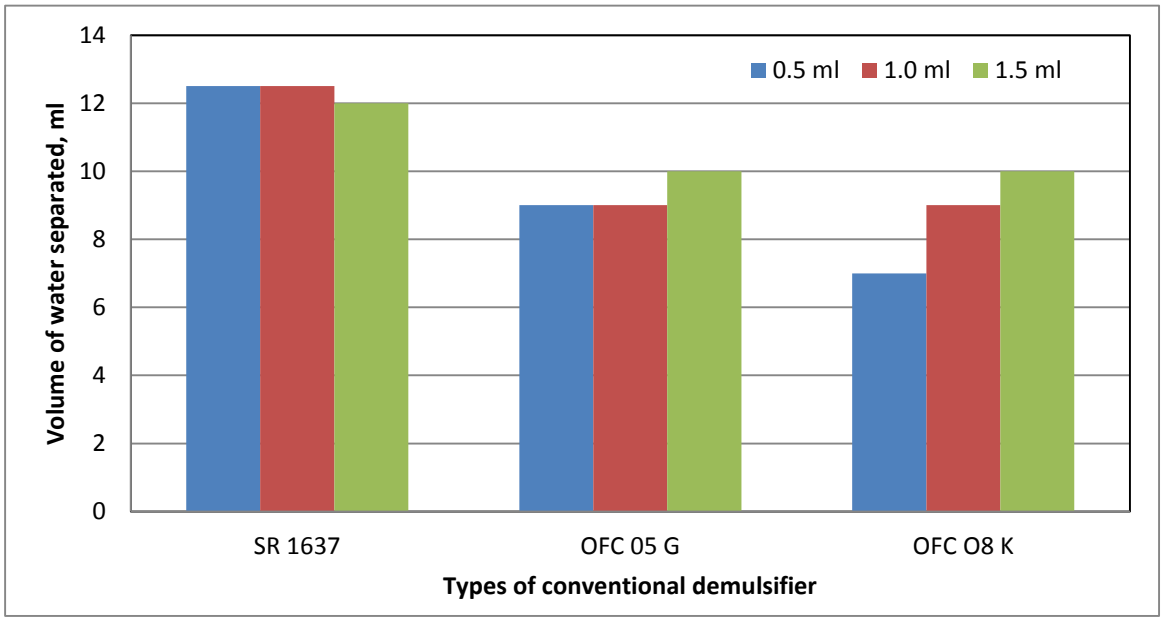


Figure 4.1 Bar chart of volume of water separated for three types of conventional demulsifier after 120 min

Based on the table and bar chart above, SR 1637 gives the best results compared with the other two conventional demulsifiers where the amount of water separated after 120 minutes is around 12.5 ml of water being separated. The water quality is also excellent as it is clear compared with the other demulsifiers that are hazy. SR 1637 is selected for further testing.

Table 4.2 Results for static bottle test of plant extract

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	E1	0.5	0	0	0	0	1	Very hazy
		1.0	0	0	0	0	1	Very hazy
		1.5	0	0	0	0	1	Very hazy
2	E2	0.5	0	9	9	9	10	Clear
		1.0	0	9	10	10	10	Clear
		1.5	0	8	9	9	10	Clear
3	E 3	0.5	0	10	10	11	11	Clear
		1.0	0	10	10	11	11	Clear
		1.5	0	10	10	11	11	Clear

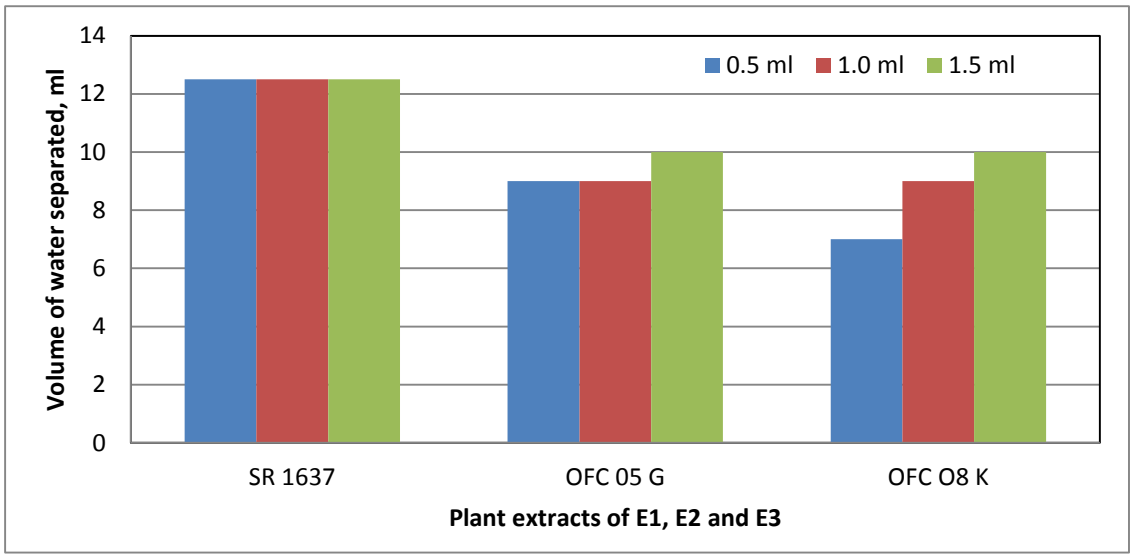


Figure 4.2 Bar chart of volume of water separated for three types of plant extracts after 120 min

Based on the table and bar chart above, E2 and E3 extracts offer better results where the final separated volume of water are 10ml and 11ml respectively for the entire dosage. The E1 extract does not show a significant impact towards the emulsion separation. The quality of water separated also is clear for E2 and E3 extract compared with the green tea extract that produce a very hazy water quality. In terms of the interface between oil and water, both E2 and E3 extracts were also able to give a sharper interface than green tea extract. This means that E2 and E3 are good dehydrating agents and are thus selected for further testing by using both plant extracts to formulate the blend demulsifier. Overall, E3 extract is the best plant extract.

Table 4.3 Results for static bottle test of blend demulsifier

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	B 1	0.5	0	5	8	8	10	Slightly hazy
		1.0	0	3	6	7	7	Slightly hazy
		1.5	0	4	6	6	7	Slightly hazy
2	B 2	0.5	0	7	10	11	11	Clear
		1.0	0	3	4	4	8	Clear
		1.5	0	2	3	3	5	Clear

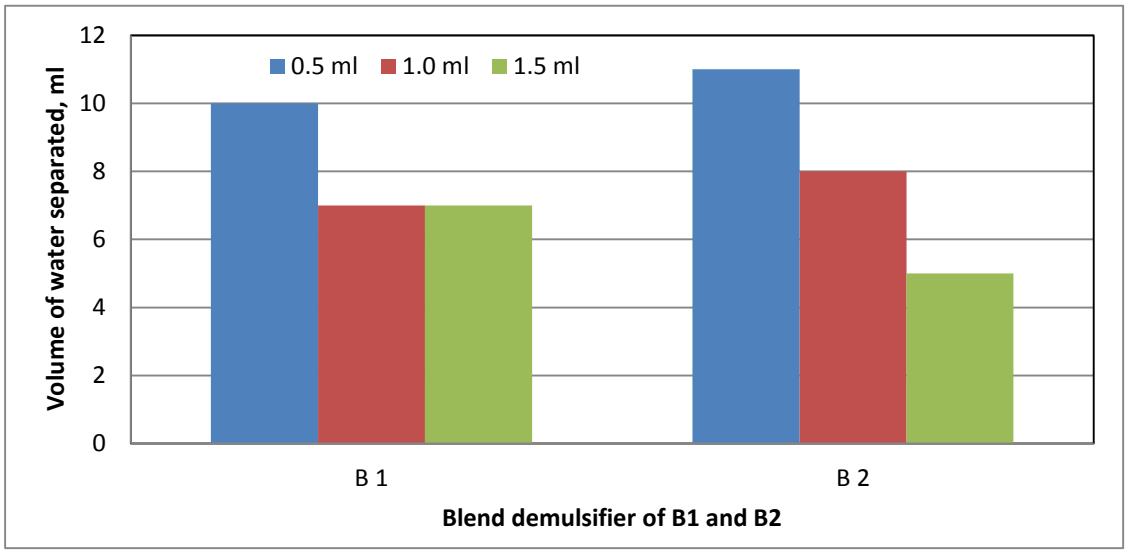


Figure 4.3 Bar chart of volume of water separated for two types of blend demulsifier after 120 min

There are two blend demulsifier formulations that have been tested that are B1, which is contained $Ca(OH)_2$ and B2 which contained NaOH. Based on the results obtained, B2 formulations have given the best results, but as the dosage is increased, the separation efficiency decreases. This is because $Ca(OH)_2$ is incompatible with the crude oil compared with NaOH. This is means that the formulation formed precipitation in the emulsion and do not spread well throughout the emulsion. This situation is good as it is economical feasible. The lower the amount of the demulsifier needed to separate water and oil effectively, the less expenditure is incurred to treat the emulsion. In terms of separated water quality, water that separated by using B2 formulations is clearer compared with B1.

Table 4.4 Results for static bottle test of blend demulsifier by using E2 extract

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	B 3	0.5	0	3	7	7	10	Clear
		1.0	0	6	7	7	7.5	Slightly hazy
		1.5	0	1	1	1	1	Slightly hazy

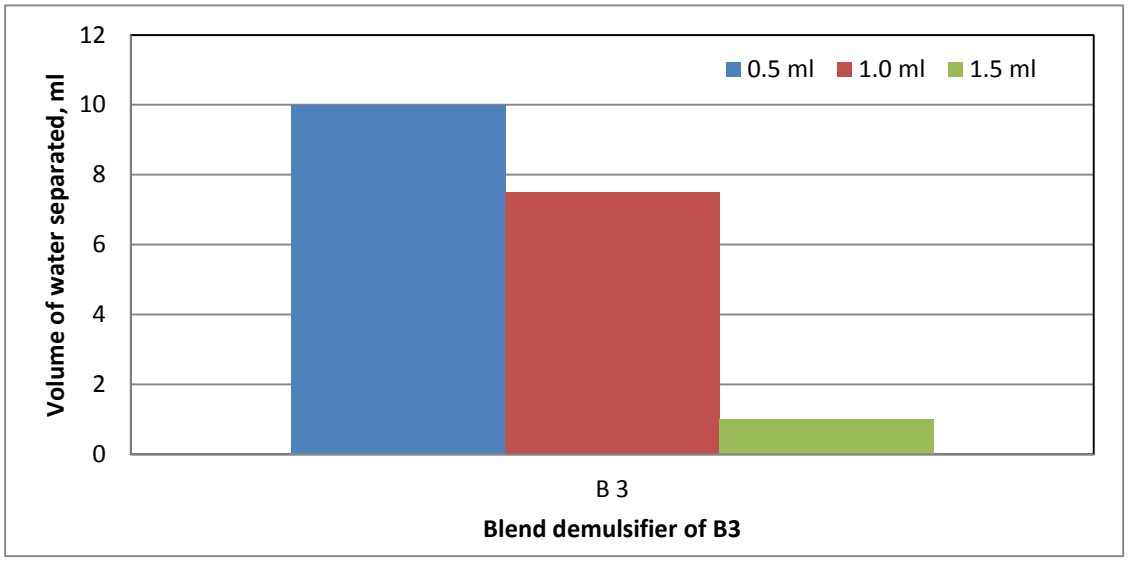


Figure 4.4 Bar chart of volume of water separated for blend demulsifier by using E2 extract after 120 min

Table and bar chart above shows the results obtained for B3. B3 is the blend formulation where the E3 extract is being replaced by E2 extract. Based on the results above, it is not promising compared with the blend demulsifier that contain E3 extract since the quality of water also is not clear for the dosage of 1 ml and 1.5 ml.

Table 4.5 Results for combination of E2 and E3

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	FE 1	0.5	0	8	9	9	11	Clear
		1.0	0	8	8	9	11	Clear
		1.5	0	7	7.5	7.5	10	Clear
2	FE 2	0.5	0	8	9	10	11	Clear
		1.0	0	7	10	11	11	Clear
		1.5	0	7	7	10	11	Clear
3	FE 3	0.5	0	8	9	9	9	Clear
		1.0	0	2	5	9	10	Slightly hazy
		1.5	0	7	8	8	8	Slightly hazy
4	FE 4	0.5	0	1	7	9	9	Clear
		1.0	0	2	5	8	9	Slightly hazy
		1.5	0	2	8	8	9	Slightly hazy
5	FE 5	0.5	0	1	6	8	8	Slightly hazy
		1.0	0	3	8	8	10	Slightly hazy
		1.5	0	5	5	8	8	Slightly hazy
6	FE 6	0.5	0	2	4	4	5	Slightly hazy
		1.0	0	3	5	5	5	Slightly hazy
		1.5	0	1	2	3	5	Slightly hazy
7	FE 7	0.5	0	7	10	10	10	Clear
		1.0	0	8	9	9	11	Clear
		1.5	0	5	7	10	11	Clear

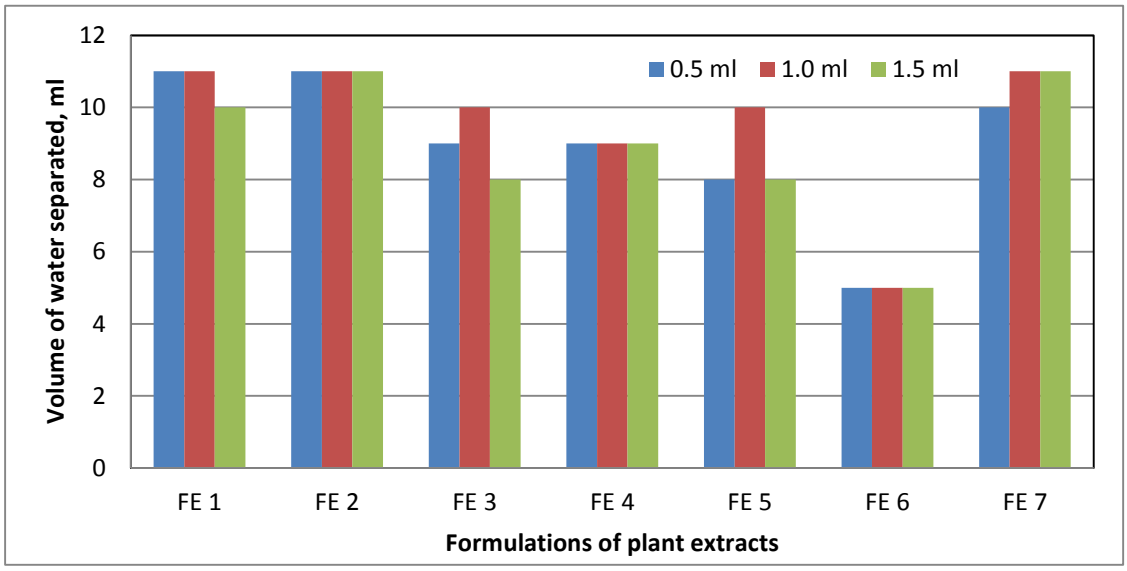


Figure 4.5 Bar chart of volume of water separated for mixture of plant extracts (E2 and E3) after 120 min

Table and bar chart above shows that the results for the formulations of E2 and E3 that mixed together in order to determine either the separation of water and oil can be enhanced further since based on the previous results that both of these extracts are very good and promising. Based on the results above, it is not consistent since these formulations only show the best result at a higher percentage of E2 or E3. For instance, the results are good for the formulations that contain 80% - 70% of E3 and 80% - 70% E2. For the formulations that contain almost half of each of the chemicals, the results are not performing well enough as these both chemicals is not compatible and not suitable to be mixed. Based on the results above, FE2 which are contain 70% of E3 and 30% of E2 give good result and the water quality also is clear.

Table 4.6 Results for combination of E3 and SR 1637

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	FI 1	0.5	0	9	10	11	11	Clear
		1.0	0	10	11	11	11	Clear
		1.5	0	9	9	10	11	Clear
2	FI 2	0.5	0	9	10	11	11	Clear
		1.0	0	7	9	9	11	Clear
		1.5	0	10	10	11	11	Clear
3	FI 3	0.5	0	8	9	10	10	Clear
		1.0	0	8	8	8	11	Clear
		1.5	0	8	9	9	10	Clear
4	FI 4	0.5	0	4	5	7	8	Clear
		1.0	0	4	5	7.5	9	Clear
		1.5	0	5	6	8	9	Clear
5	FI 5	0.5	0	5	7	9	9	Clear
		1.0	0	7	8	10	10	Clear
		1.5	0	5	6	8	8	Slightly hazy
6	FI 6	0.5	0	8	9	10	10	Clear
		1.0	0	9	9	10	10	Clear
		1.5	0	9	9	9	10	Clear
7	FI 7	0.5	0	5	6	8	9	Clear
		1.0	0	7	7	9	9	Clear
		1.5	0	7	7	10	11	Clear

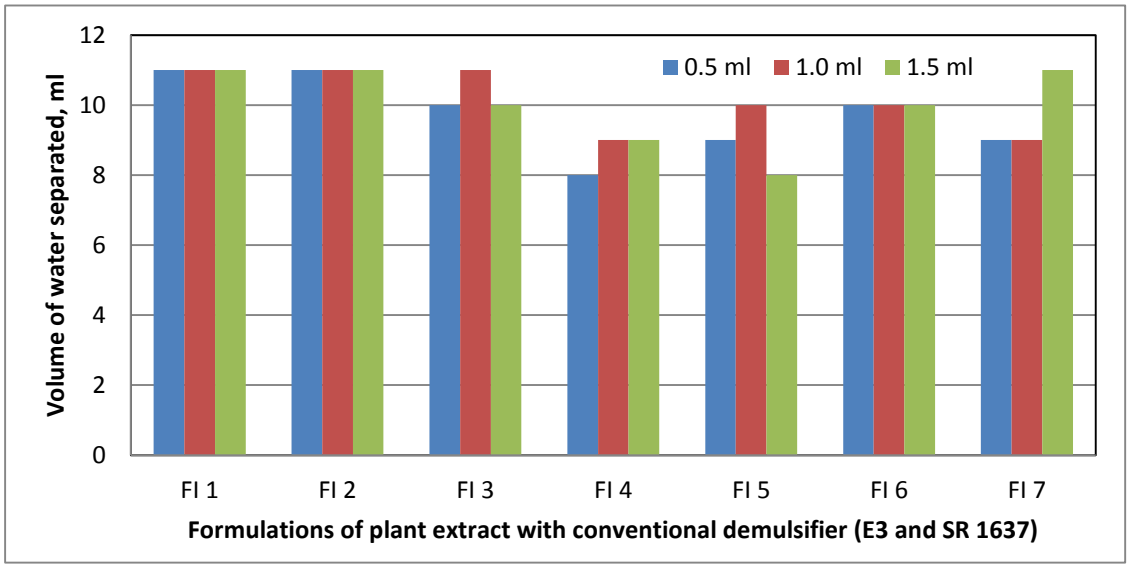


Figure 4.6 Bar chart of volume of water separated for mixture of plant extracts with conventional demulsifier (E3and SR 1637) after 120 min

Table and bar chart above shows the formulations for the combination of the best green demulsifier, E3 with the best conventional demulsifier, SR 1637. The results obtained are almost same with the results in the previous table where it is good for the formulations that contain 80% - 70% of E3 and 80% - 70% of SR 1637. For the formulations that contain almost half of each of the chemicals, the results are also not performing well enough as these both chemicals is not compatible and not suitable to be mixed. Based on the results above, FI1 which are contain 80% of E3 and 20% of SR 1637 shows good result and the water quality also is clear.

Table 4.7 Results for the best demulsifier formulations

No.	Product	Demulsifier dosage (ml)	Volume of separated water (ml)					Water quality
			0 min	10 min	30 min	60 min	120 min	
1	SR 1637	0.5	0	9	11	12	12.5	Clear
		1.0	0	9	12	12	12.5	Clear
		1.5	0	10	10	11	12	Clear
2	E 2	0.5	0	9	9	9	10	Clear
		1.0	0	9	10	10	10	Clear
		1.5	0	8	9	9	10	Clear
3	E 3	0.5	0	10	10	11	11	Clear
		1.0	0	10	10	11	11	Clear
		1.5	0	10	10	11	11	Clear
4	B 2	0.5	0	7	10	11	11	Clear
		1.0	0	3	4	4	8	Clear
		1.5	0	2	3	3	5	Clear
5	FE 2	0.5	0	8	9	10	11	Clear
		1.0	0	7	10	11	11	Clear
		1.5	0	7	7	10	11	Clear
6	FI 1	0.5	0	9	10	11	11	Clear
		1.0	0	10	11	11	11	Clear
		1.5	0	9	9	10	11	Clear

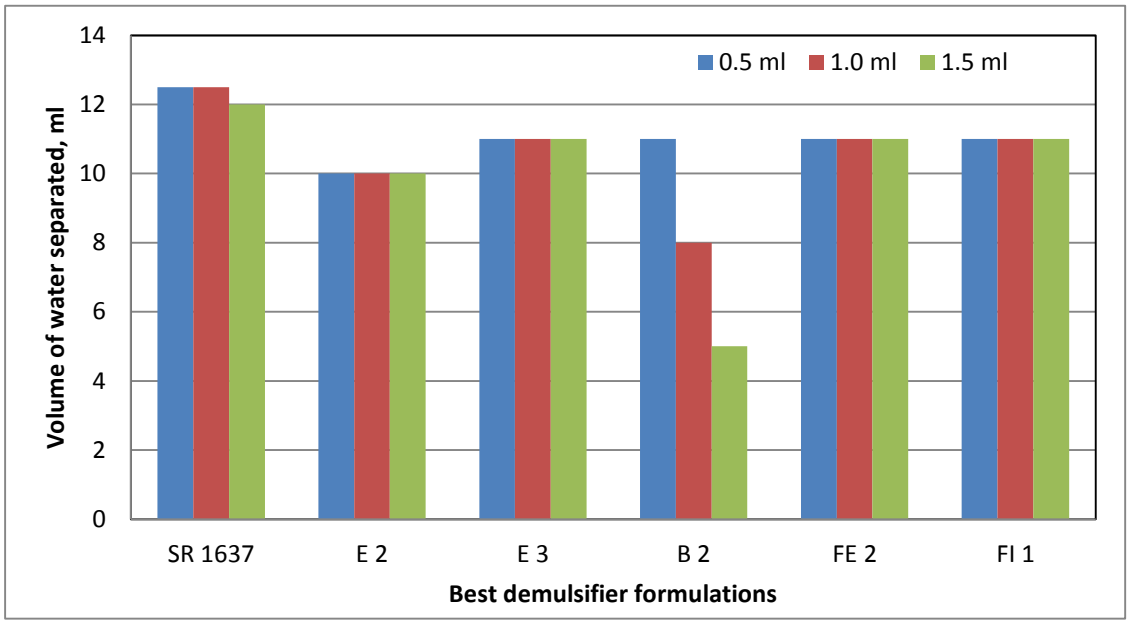


Figure 4.7 Bar chart of volume of water separated for the best demulsifier formulations after 120 min

Table and bar chart above shows the results of volume of water separated for six best demulsifier formulations that are SR 1637, E2, E3, B2 FE2 and FI 1. SR 1637 is not selected for the final formulations since it is from industry and is highly toxic. Based on the results, E3, FE 2 and FI 1 give the best results that are around 11 ml of water separated after 120 minutes for all dosages. These best three demulsifiers will further analyzed based on the dosages and the volume of water separated at 0 minute, 10 minutes, 30 minutes, 60 minutes and 120 minutes.

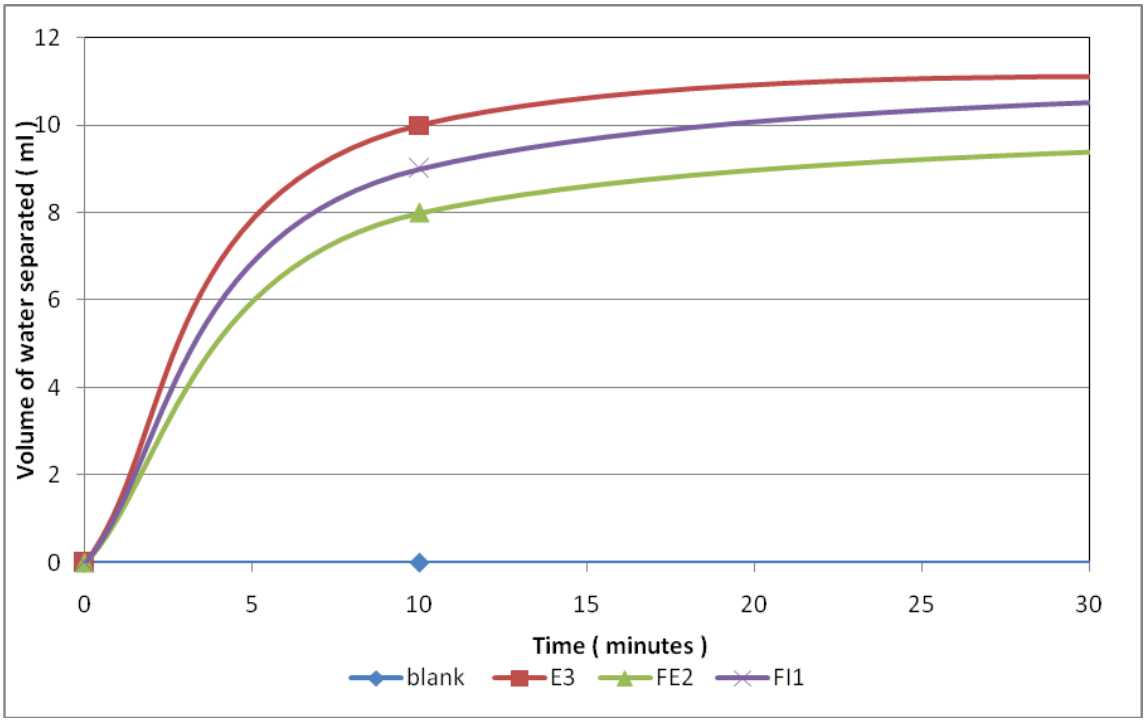


Figure 4.8 Graph of volume of water separated (ml) against time (min) for the best demulsifier formulations for 0.5 ml

Graph above shows that the volume of water separated within 10 minutes of time for demulsifier dosage of 0.5 ml as the normal time allocated for the emulsion to separate in the system is only 10 minutes and below. Based on the graph above, E3 gives a good performance that is around 10 ml of water separated compared with FE2 and FI1which can separate the water for about 9 ml and 8 ml. Based on the industry condition, E3 shows the best results within 10 minutes as it can squeeze out the water for about 90%.

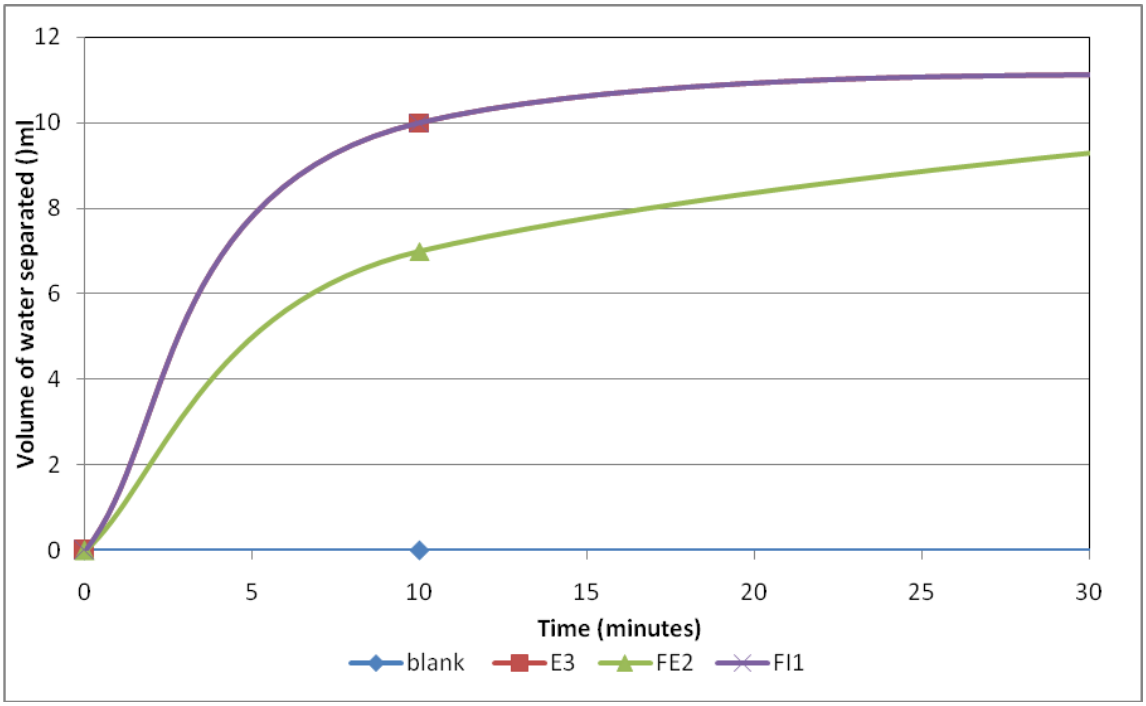


Figure 4.9 Graph of volume of water separated (ml) against time (min) for the best demulsifier formulations for 1.0 ml

Graph above shows that the volume of water separated within 10 minutes of time for demulsifier dosage of 1.0 ml. The results show different trending with the previous results. As 1 ml of demulsifiers added into the emulsion, E3 and FI 1 give good results as the water separated from both demulsifiers is 10 ml and the result for FI 2 is going down from 8 ml to 7 ml. This is because the amount of the demulsifier has exceed the point of injection amount and the exceess amount will the cause the demulsifier to coagulate and do not spread well throughout the emulsion. The results for this demulsifier will be decreases if the amount of the chemical is increased.

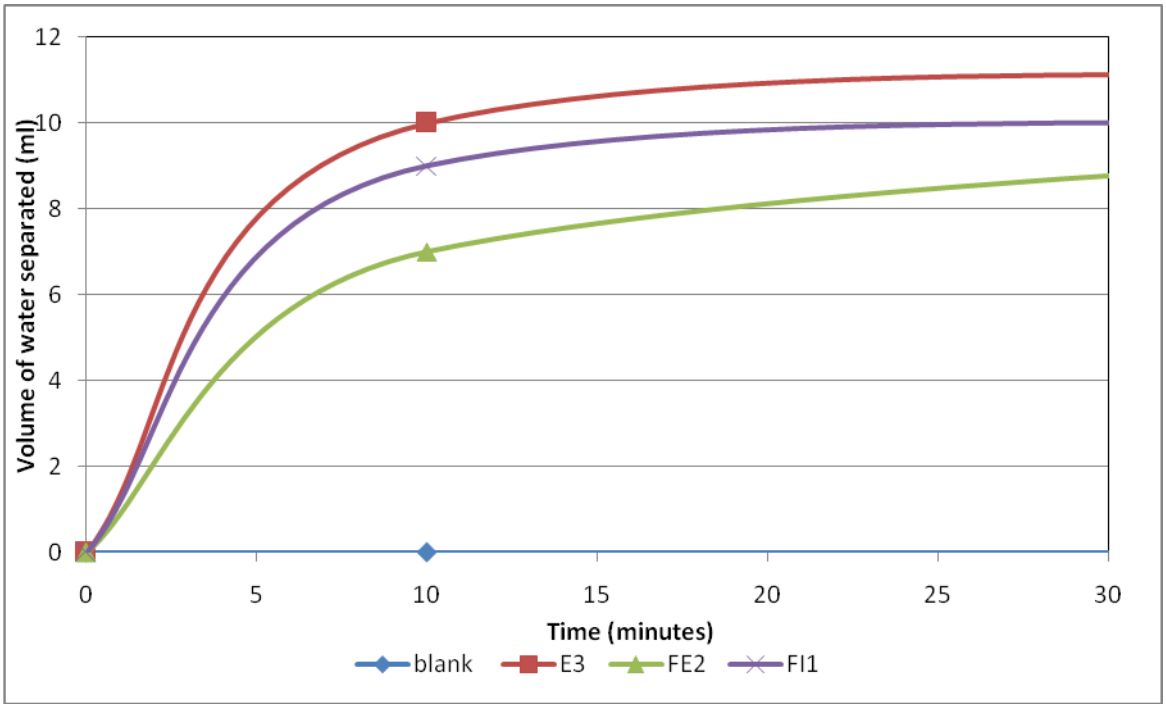


Figure 4.10 Graph of volume of water Separated (ml) against time (min) for the best demulsifier formulations for 1.5 ml

Graph above clearly shows that E3 give the best performance compared with FE 2 and FI1. It can be finalized that E3 individually is the best extract that can separate water and oil as it is able to act as a surfactant and also as an interface corrector. Meanwhile, FI 1 is the second option or second candidate to be selected as green demulsifier as the results for all dosages of FI1 is not stable. This is because, this demulsifier is formulated by two types of plant extracts and the extracts is not well mixed due to the different in density and immiscible. As the demulsifier in added into the emulsion, the extracts is reacted individually with the emulsion in their own way. Based on these both demulsifiers, E3 is the most suitable demulsifier to be selected as it is likely to have the lowest toxicity level as it is 100% organic. Meanwhile, FI 1 was blended with some amount of SR 1637 that contain highly toxic. The analysis of toxicity level can be seen in the toxicity level test.

4.2 Dynamic Bottle Test

Table 4.8 Results for demulsifier formulations for dynamic bottle test

No	Products	Demulsifier dosage, ml			Water quality
		0.5	1	1.5	
Conventional demulsifier					
1	SR 1637	8	11	11	Clear
2	OFC 05 G	3	3	6	Clear
3	OFC 08 K	3	5	6	Clear
Plant extracts					
4	E 1	1	1	3	Clear
5	E 2	8	7	10	Clear
6	E 3	10	11	11	Clear
Blend demulsifier					
7	B 1	5	6	6	Clear
8	B 2	8	7	5	Clear
9	B 3	5	5	3	Clear
Formulations of two best plant extracts					
10	FE 1	9	10	8	Clear
11	FE 2	9	10	10	Clear
12	FE 3	5	5	7	Clear
13	FE 4	5	4	6	Clear
14	FE 5	6	8	6	Clear
15	FE 6	3	5	7.5	Clear
16	FE 7	5	6	8	Clear
Formulation of plant extract with conventional demulsifier					
17	FI 1	8	10	10	Clear
18	FI 2	7	9	10	Clear
19	FI 3	6	7	8	Clear
20	FI 4	6	7	7.5	Clear
21	FI 5	4	5	4	Clear
22	FI 6	7	9	9	Clear
23	FI 7	7	7	7.5	Clear

Table above shows the results of the demulsifier formulations that have been tested in dynamic condition test by using a bench centrifuge for 10 minutes. Similar with the static bottle test, the test is divided into several groups which are conventional demulsifier group, plant extract group, blend demulsifier group, formulation of plant extract group and finally is the group of formulation of a plant extract with conventional demulsifier. The formulations that give the best result from each group is selected for further analysis. Based on the table above, there are six best formulations that give good results which are SR 1637, E2, E3, B2, FE2 and FI 1.

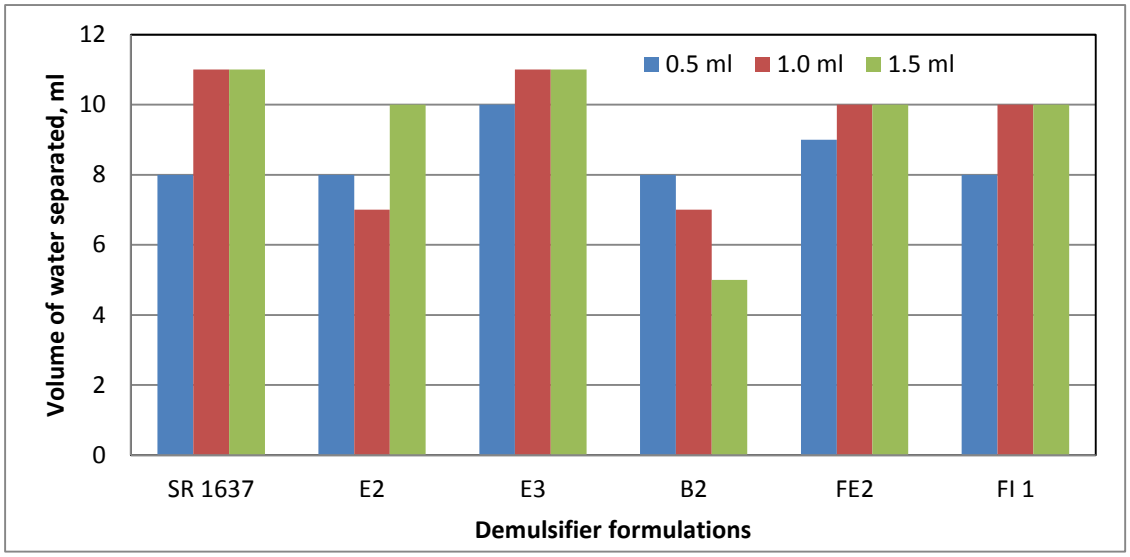


Figure 4.11 Bar chart of volume of water separated for the best demulsifier

Figure above shows the results of the best demulsifier formulations for dynamic bottle test. Based on the bar chart, it is obviously that SR 1637 and E3 are the best demulsifiers as they are able to separate the water almost 85% to 90%. SR 1637 is not selected in this project as it is highly toxic and automatically E3 formulation is selected as the best green demulsifier same with the static bottle test.

4.3 Results for Plant Extract Compositions Identification

Identification the compositions of plant extracts is done by using Gas Chromatography-Mass Spectrometer (GC-MS). Based on the results obtained, all of the plant extracts contain high fatty acid, naphthenic acid and polyphenols compositions that can reduce the interfacial tension energy. There are about 5.553% of hexane and 3.000% of Octadecenoic acid composition in E1 extracts. Meanwhile, in E2 extracts, there are 33.943% of hexane and 9.106% of Octadecenoic acid group compositions. E3 extract contains about 1.787% of hexane and 3.642% of Octadecenoic acid. There are also other compositions that contain in these plants but not much of them. Full results for plant extract composition identification is provided in the APPENDIX III indicated by GTE for green tea extract, OOE for olive extract and CE for coconut extract.

4.4 Analysis of Toxicity Level of the Best Demulsifier Formulations

Table 4.9 Toxicity levels of the best demulsifier formulations

No	Products	SR 1637	E 2	E 3	B 2	FE 2	FI 1
1	Time for the fish to die, min	10	107	110	8	90	60
2	pH value	 pH = 3	 pH = 6	 pH = 6	 pH = 12	 pH = 5	 pH = 5

Table above shows the results of the toxicity level test by observing the effect of the demulsifiers on the fish by monitoring the time taken for the fish to die and the pH value of the chemicals. The fishes are placed in different containers filled with water injected

with different demulsifiers. Based on the table, the time taken for the fish that placed in container that injected with SR 1637 and B2 were taking short time to die which are only 10 minutes and 8 minutes respectively as both demulsifiers are highly toxic. B2 is containing NaOH and has alkali property. Meanwhile, fishes that are placed in the container that filled with water that injected with E2 and E3 is longer time to die. This is because the pH value of these demulsifiers is almost neutral that is around 6 to 7.

The acidity and alkalinity of these demulsifiers can be confirmed by using litmus paper. The results that obtained from the pH test show that SR 1637 have a pH value of 3 that is high acidic and the pH value for B2 is 12 that is high alkali content. Meanwhile, the pH value for both E2 and E3 is 6 that are almost neutral.

High pH levels which is 9 to 14 can harm fish by denaturing cellular membrans. This is because, most ammonium that contain in the water is converted to toxic ammonia. Meanwhile, if the pH of the water is too low, the metals from the rock or sediments in the stream is released rapidly and these metals can affect the fish's metabolism and disrupt the water flow in through the gills and can kill fish fry.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

As a conclusion, this project has focused on the breaking of the emulsion crude in order to increase the oil recovery by using demulsifier with respect to the environmental issue. The author used three types of plants which are green tea leaves (E1), olive (E2), and coconut (E3) extracts by considering all the compositions and the capability in resolving emulsion. In order to develop and complete the performance assessment, static bottle tests and dynamic bottle test are carried out. There are four parameters that are evaluated, the amount of the water separated, the quality of the water separated, the separation time between water and oil and the amount of demulsifier used.

Based on the results obtained, the author has concluded that E3 extract is the best extract that can separate oil and water effectively within the time range and also able to show clear water which means that maximum amount of water is extracted from the oil. This E3 extract cannot be added or mixed with other extracts for formulation as the effectiveness is reduced. This is because, E3 extract is not compatible enough to be tested together with other extracts or formulations as the interface that formed is not sharp and the water separation also is not at the maximum level.

5.2 Recommendation

There are three recommendations of this project for future improvement. In order to find the best plant extracts, different parts of plants can be used such as the leaves part, fruit, seed and bark since each part of the plants contains different chemical compositions.

The second recommendation for this project is regarding the synthetic emulsion formulation. In this project, the author only uses 50%-50% of synthetic emulsion formulations. For future development, the author recommends for different formulations such as, 80%-20% (80% oil +20% water) and 30%-70% (30% oil + 70% water) in order to see the effectiveness of the plant extracts towards different formulations of emulsion.

In order to get more reliable results, the static and dynamic test can be conducted by using the actual crude emulsion sample from the actual field. That kind of emulsion can be requested from the industrial companies. The test also should be conducted at different temperatures where ranging from 50°C until 65°C since the operating temperature at the real field is between this range.

The third recommendation is to determine the toxicity level of the demulsifier by measuring the parameters like molecular weight, log kow, henry's law constant and vapour pressure instead of measuring the pH value of the demulsifiers.

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APPENDIX A

Table A-1: Demulsifier formulations design

No.	Experimental code	Formulation
1	E1	Plant extract for green tea
2	E2	Plant extract for olive
3	E3	Plant extract for coconut
4	B1	10% E3+ 10% Starch + 20% Camphor + 20% Ca(OH)2 + 20% Paraffin wax + 20% Liquid Soap
5	B2	10% E3 + 10% Starch + 20% Camphor + 20% NaOH + 20% Paraffin wax + 20% Liquid Soap
6	B3	10% E2 + 10% Starch + 20% Camphor + 20% NaOH + 20% Paraffin wax + 20% Liquid Soap
9	FE1	80% E3 + 20% E2
10	FE2	70% E3 + 30% E2
11	FE3	60% E3 + 40% E2
12	FE4	50% E3 + 50% E2
13	FE5	40% E3 + 60% E2
14	FE6	30% E3 + 70% E2
15	FE7	20% E3 + 80% E2
16	FI1	80% E3 + 20% SR 1637
17	FI2	70% E3 + 30% SR 1637
18	FI3	60% E3 + 40% SR 1637
19	FI4	50% E3 + 50% SR 1637
20	FI5	40% E3 + 60% SR 1637
21	FI6	30% E3 + 70% SR 1637
22	FI7	20% E3 + 80% SR 1637

APPENDIX B

Results for Three Best Demulsifier Formulations

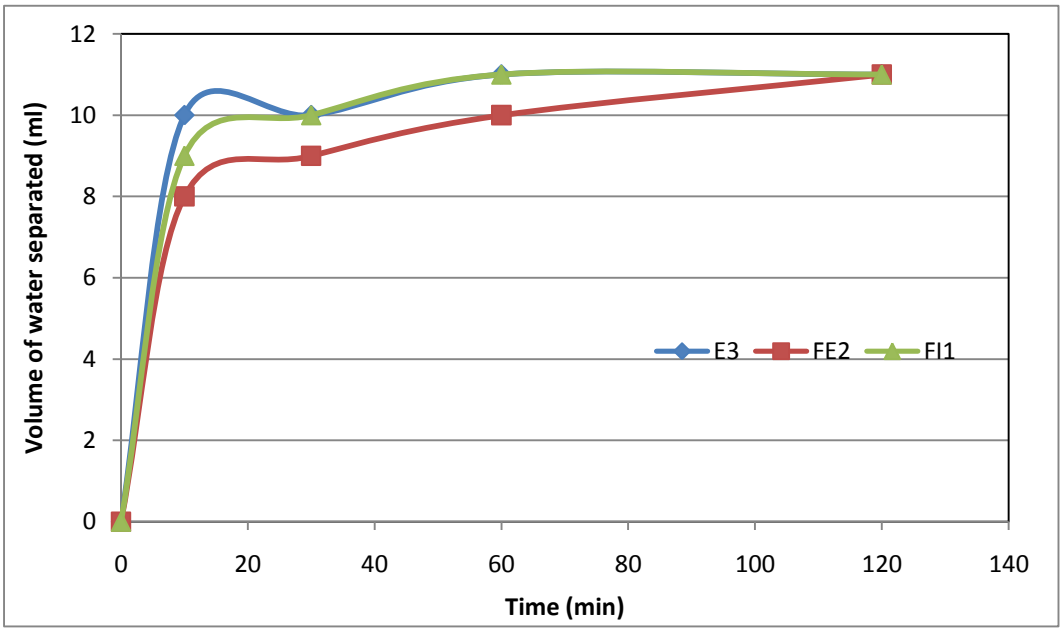


Figure B-1 Graph of volume of water separated (ml) against time (min) for the best demulsifier formulations for 0.5 ml

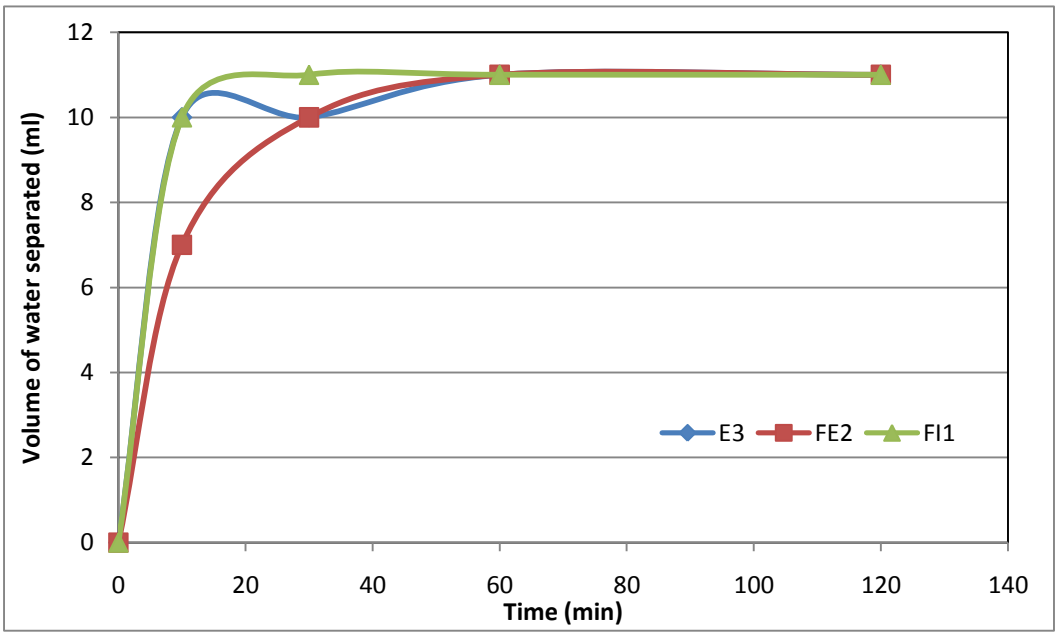


Figure B-2 Graph of volume of water separated (ml) against time (min) for the best demulsifier formulations for 1.0 ml

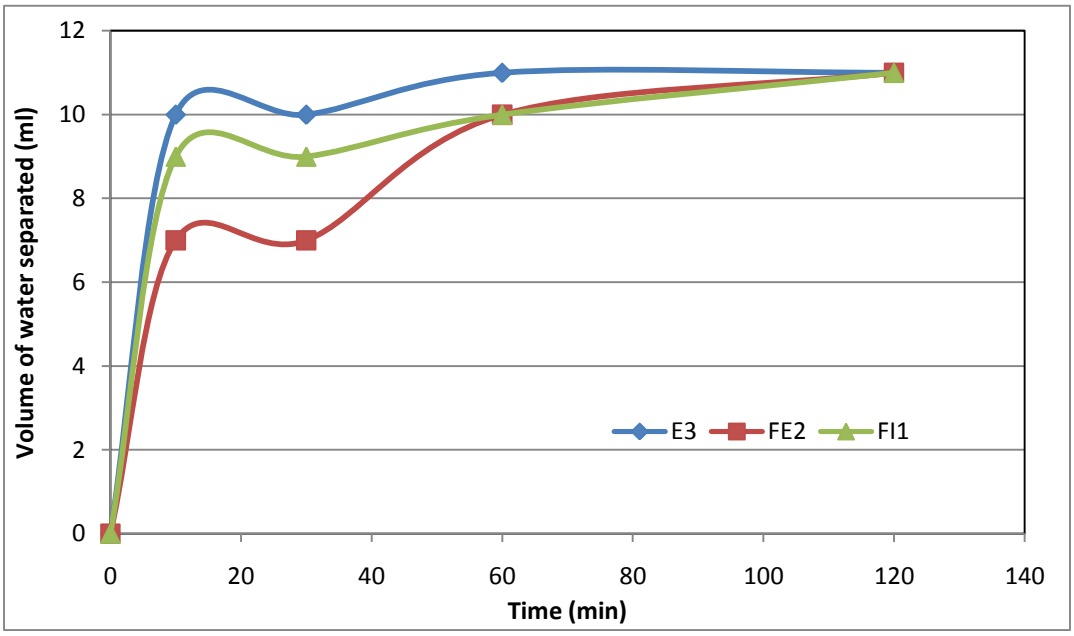
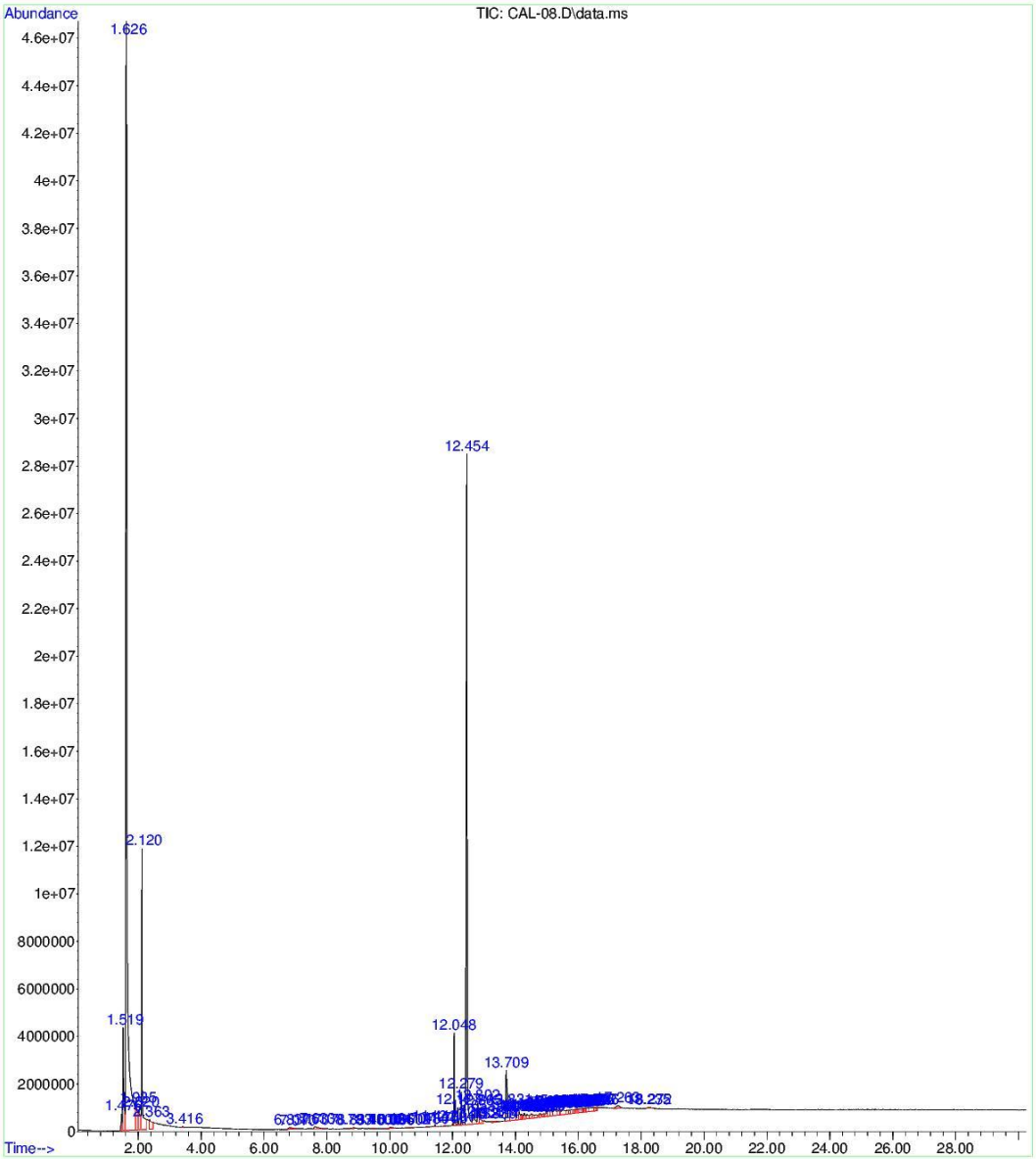


Figure B-3 Graph of volume of water separated (ml) against time (min) for the best demulsifier formulations for 1.5 ml

APPENDIX C

Full Results for Plant Extracts Compositions Identification

```
File       :C:\msdchem\CAL 2010\DATA\2014\Yaakob\CAL-08.D
Operator   : Hasbullah
Acquired   : 12 Jul 2014  14:27     using AcqMethod BOIL-001NORIZAN.M
Instrument :   gcms1
Sample Name: GTE
Misc Info  :
Vial Number: 3
```



Area Percent Report

Acq On : 12 Jul 2014 14:27

Sample : GTE
Data File : CAL-08.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Integration Parameters: genie.e

Signal : TIC: CAL-08.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	204	215	218	BV 2	681239	13609371	0.97%	0.469%
2	1.519	218	221	231	VV	4233821	95082603	6.75%	3.275%
3	1.626	231	238	283	VV 3	47159794	1408601666	100.00%	48.524%
4	1.935	283	286	296	VV	1028179	43745043	3.11%	1.507%
5	2.020	296	299	309	VV	812752	33861634	2.40%	1.166%
6	2.120	309	314	337	VV	10655311	161194724	11.44%	5.553%
7	2.363	348	352	368	VV 3	405293	24696375	1.75%	0.851%
8	3.416	511	515	517	PV	37772	347629	0.02%	0.012%
9	6.837	1027	1043	1068	PV 6	67247	5708023	0.41%	0.197%
10	7.010	1068	1070	1072	VV 3	5458	63005	0.00%	0.002%
11	7.633	1155	1166	1176	VV 3	99281	5058994	0.36%	0.174%
12	7.707	1176	1178	1213	VV 3	60431	3841947	0.27%	0.132%
13	8.783	1334	1344	1347	VV 10	41926	1158994	0.08%	0.040%
14	8.837	1347	1353	1356	VV 8	37761	1286208	0.09%	0.044%
15	9.450	1444	1447	1457	VV 2	38432	610715	0.04%	0.021%
16	10.024	1521	1536	1539	PV 2	42888	1325811	0.09%	0.046%
17	10.051	1539	1540	1544	VV 4	31356	535979	0.04%	0.018%
18	10.096	1544	1547	1556	VV 10	30793	784249	0.06%	0.027%
19	10.602	1618	1626	1630	PB 8	14570	150490	0.01%	0.005%
20	10.707	1638	1642	1645	PV 3	25864	272318	0.02%	0.009%
21	11.180	1711	1715	1717	PV 5	23976	254137	0.02%	0.009%
22	11.442	1750	1755	1766	PV	98070	1325887	0.09%	0.046%
23	11.758	1796	1804	1809	PV	31588	624936	0.04%	0.022%
24	12.004	1838	1842	1845	PV	77567	854880	0.06%	0.029%
25	12.048	1845	1849	1865	VV	3911538	46663507	3.31%	1.607%
26	12.177	1865	1869	1880	VV	753069	10091655	0.72%	0.348%
27	12.279	1880	1885	1901	VV	1327559	15544552	1.10%	0.535%
28	12.454	1901	1912	1937	VV	27620107	584254907	41.48%	20.127%
29	12.653	1937	1943	1960	VV	424651	19184683	1.36%	0.661%
30	12.802	1960	1966	1973	VV	829982	20781911	1.48%	0.716%
31	12.865	1973	1975	1984	VV	578433	12528105	0.89%	0.432%
32	12.933	1984	1986	1993	VV 7	134634	3867458	0.27%	0.133%
33	13.277	2031	2039	2043	VV 10	48956	1396046	0.10%	0.048%
34	13.330	2043	2047	2050	VV 6	38515	729163	0.05%	0.025%
35	13.414	2054	2060	2065	VV 10	37196	1011506	0.07%	0.035%
36	13.709	2092	2106	2123	PV 2	2107628	87091169	6.18%	3.000%
37	13.831	2123	2125	2153	VV 7	542335	38224090	2.71%	1.317%
38	14.025	2153	2155	2165	VV 7	224149	9617149	0.68%	0.331%
39	14.123	2165	2170	2177	VV 3	324905	10759846	0.76%	0.371%
40	14.193	2177	2181	2184	VV	226209	4824357	0.34%	0.166%
41	14.226	2184	2186	2189	VV 4	184373	3733598	0.27%	0.129%
42	14.280	2189	2194	2202	VV	248038	8757413	0.62%	0.302%
43	14.367	2202	2208	2218	VV	191341	9206121	0.65%	0.317%

44	14.503	2218	2228	2232	VV		184673	8664185	0.62%	0.298%
45	14.535	2232	2234	2242	VV	9	165040	5397652	0.38%	0.186%
46	14.657	2242	2252	2258	VV	9	125535	7356083	0.52%	0.253%
47	14.784	2265	2272	2276	VV	8	152701	5182805	0.37%	0.179%
48	14.889	2282	2288	2291	VV	8	129285	3940129	0.28%	0.136%
49	14.921	2291	2293	2296	VV	4	118035	2379561	0.17%	0.082%
50	14.997	2296	2305	2309	VV	6	240231	7912017	0.56%	0.273%
51	15.050	2309	2313	2321	VV	3	281657	11477571	0.81%	0.395%
52	15.119	2321	2324	2334	VV		252412	11187988	0.79%	0.385%
53	15.237	2334	2342	2357	VV	9	305646	18783709	1.33%	0.647%
54	15.376	2357	2363	2369	VV	9	179061	7686669	0.55%	0.265%
55	15.432	2369	2372	2374	VV	4	155047	3121940	0.22%	0.108%
56	15.526	2374	2387	2397	VV	4	187671	15229141	1.08%	0.525%
57	15.646	2397	2405	2411	VV	4	155057	8106971	0.58%	0.279%
58	15.716	2411	2416	2420	VV	7	154212	5029985	0.36%	0.173%
59	15.809	2420	2430	2433	VV	7	163906	7811813	0.55%	0.269%
60	15.835	2433	2434	2441	VV	7	158639	5017883	0.36%	0.173%
61	15.890	2441	2443	2444	VV	2	151817	1843078	0.13%	0.063%
62	15.914	2444	2447	2449	VV	4	154254	2815693	0.20%	0.097%
63	15.952	2449	2453	2456	VV	6	159955	4042724	0.29%	0.139%
64	16.004	2456	2461	2462	VV	4	158373	3664981	0.26%	0.126%
65	16.035	2462	2465	2473	VV	10	158097	6209272	0.44%	0.214%
66	16.108	2473	2477	2480	VV	6	163412	4709224	0.33%	0.162%
67	16.148	2480	2483	2484	VV	3	158920	2261303	0.16%	0.078%
68	16.178	2484	2488	2490	VV	4	160900	3836832	0.27%	0.132%
69	16.229	2490	2495	2497	VV	6	163387	4153023	0.29%	0.143%
70	16.324	2497	2510	2512	VV	6	151593	8370477	0.59%	0.288%
71	16.436	2512	2527	2536	VV	6	158820	14407234	1.02%	0.496%
72	16.502	2536	2538	2547	VV	9	146475	5675461	0.40%	0.196%
73	16.586	2547	2551	2554	VV	6	132685	3709245	0.26%	0.128%
74	17.263	2634	2655	2672	VV	5	108603	9005003	0.64%	0.310%
75	18.235	2800	2805	2807	PV	5	12443	248145	0.02%	0.009%
76	18.272	2807	2811	2818	VV	9	18289	410248	0.03%	0.014%

Sum of corrected areas: 2902910897

B-OIL.M Wed Jul 16 09:42:36 2014

Library Search Report

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Data File : CAL-08.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Search Libraries: C:\Database\NIST08.L Minimum Quality: 50

Unknown Spectrum: Apex minus start of peak
Integration Events: ChemStation Integrator - genie.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.478	0.47	C:\Database\NIST08.L			
			Dasycarpidan-1-one	111838	002825-08-3	46
			1,3-Dioxolane-4-methanol	4650	005464-28-8	43
			Fluoxetine	143330	054910-89-3	38
2	1.517	3.28	C:\Database\NIST08.L			
			Methyl Alcohol	31	000067-56-1	2
			Methyl Alcohol	29	000067-56-1	2
			Adenosine, 2-methyl-	121459	016526-56-0	2
3	1.627	48.52	C:\Database\NIST08.L			
			Ethanol	95	000064-17-5	9
			Hydrazine, methyl-	101	000060-34-4	9
			Hydrazine, methyl-	103	000060-34-4	9
4	1.937	1.51	C:\Database\NIST08.L			
			Pentane, 2-methyl-	1814	000107-83-5	72
			Pentane, 2-methyl-	1816	000107-83-5	59
			Pentane, 3,3-dimethyl-	3954	000562-49-2	37
5	2.022	1.17	C:\Database\NIST08.L			
			Pentane, 3-methyl-	1817	000096-14-0	64
			Pentane, 3-methyl-	1815	000096-14-0	64
			Pentane, 3-methyl-	1818	000096-14-0	38
6	2.119	5.55	C:\Database\NIST08.L			
			Hexane	1812	000110-54-3	94
			Hexane	1811	000110-54-3	91
			Hexane	1813	000110-54-3	91
7	2.364	0.85	C:\Database\NIST08.L			
			Cyclopentane, methyl-	1487	000096-37-7	80
			Cyclohexane	1452	000110-82-7	80
			1H-Tetrazole, 5-methyl-	1323	004076-36-2	64
8	3.419	0.01	C:\Database\NIST08.L			
			Ethane, 1,1-diethoxy-	8734	000105-57-7	53
			Ethane, 1,1-diethoxy-	8730	000105-57-7	50
			Butane, 2-ethoxy-	4389	002679-87-0	37
9	6.834	0.20	C:\Database\NIST08.L			
			2(1H)-Pyridinone, 6-hydroxy-	6018	000626-06-2	53
			Imidazole-4-carboxamide	5991	026832-08-6	43
			1,2,5,6-Tetrahydropyridin-2-one, 5-methyl-	6074	1000197-00-2	42
10	7.009	0.00	C:\Database\NIST08.L			
			2-Butyndiol dimethyl ether	7143	016356-02-8	32
			6-Aminotetrazolo(b)pyridazine	15754	019195-43-8	17
			2,6-Dinitrobenzonitrile	54011	035213-00-4	10
11	7.630	0.17	C:\Database\NIST08.L			

		2-Cyclopentene-1,4-dione	2722	000930-60-9	35
		2-Cyclopentene-1,4-dione	2720	000930-60-9	35
		2(1H)-Pyrimidinone, 4-amino-	6003	000071-30-7	35
12	7.707	0.13 C:\Database\NIST08.L			
		2-Ethyl-cyclohexylamine	11762	024216-90-8	50
		2,5-Pyrrolidinedione, 1-ethyl-	11639	002314-78-5	40
		Phosphonofluoridic acid, (1-methyl ethyl)-, ethyl ester	26719	001426-08-0	37
13	8.781	0.04 C:\Database\NIST08.L			
		Benzofuran, 2,3-dihydro-	9283	000496-16-2	35
		Benzenamine, N-ethyl-N-methyl-	15434	000613-97-8	25
		Benzonitrile, 2-hydroxy-	9024	000611-20-1	25
14	8.839	0.04 C:\Database\NIST08.L			
		Benzaldehyde, 2-methyl-	9271	000529-20-4	76
		Benzaldehyde, 4-methyl-	9272	000104-87-0	76
		Benzaldehyde, 3-methyl-	9276	000620-23-5	76
15	9.447	0.02 C:\Database\NIST08.L			
		Tetradecane	58108	000629-59-4	76
		Pentadecane	68976	000629-62-9	64
		Undecane, 5,7-dimethyl-	47645	017312-83-3	64
16	10.023	0.05 C:\Database\NIST08.L			
		Benzamide, N-(2-piperidinylmethyl)-2,5-bis(2,2,2-trifluoroethoxy)-	199541	054143-55-4	72
		Piperidine, 2-propyl-, (S)-	11776	000458-88-8	64
		Pidolic Acid	12679	000098-79-3	64
17	10.049	0.02 C:\Database\NIST08.L			
		1-Propene, 3,3,3-trifluoro-2-methyl-	5613	000374-00-5	12
		Benzene, 1,3,5-trichloro-2-nitro-	78924	018708-70-8	12
		4-Benzofurazanamine, 7-nitro-N-phenyl-	102158	018378-15-9	12
18	10.094	0.03 C:\Database\NIST08.L			
		Dodecane, 5,8-diethyl-	79892	024251-86-3	47
		Undecane	27917	001120-21-4	43
		Undecane	27916	001120-21-4	43
19	10.605	0.01 C:\Database\NIST08.L			
		1H-Pyrrole-2-carboxylic acid, 1-ethenyl-	16488	034600-55-0	42
		Phenol, 4-amino-2,5-dimethyl-	16550	003096-71-7	42
		2,5-Cyclohexadien-1-one, 4,4-dimethoxy-3-methyl-	36547	072054-83-2	35
20	10.709	0.01 C:\Database\NIST08.L			
		Hexadecane	79880	000544-76-3	70
		Hexadecane	79878	000544-76-3	55
		Hexadecane	79879	000544-76-3	55
21	11.181	0.01 C:\Database\NIST08.L			
		1-Tridecene	46097	002437-56-1	86
		6-Tridecene, (Z)-	46110	006508-77-6	70
		4-Tridecene, (Z)-	46101	041446-54-2	64
22	11.440	0.05 C:\Database\NIST08.L			
		1-Nonanol, 4,8-dimethyl-	38922	033933-80-1	72
		1-Dodecanol, 3,7,11-trimethyl-	81361	006750-34-1	64
		3-Nonene, (E)-	11389	020063-92-7	62
23	11.757	0.02 C:\Database\NIST08.L			
		4-Nonene, 5-butyl-	46113	007367-38-6	55
		Cyclopropane, 1-(1,2-dimethylpropyl)-1-methyl-2-nonyl-	99576	041977-42-8	52
		1,4-Bis(trifluoroacetyl)-3,6-bis(1	200625	1000281-06-7	38

```
                -methylpropyl)-2,5-diketopiperazin

24  12.003  0.03 C:\Database\NIST08.L
                2-Hexadecene, 3,7,11,15-tetramethy 121355 014237-73-1 93
                l-, [R-[R*,R*-(E)]]-
                1-Decene                            17712 000872-05-9 72
                Cyclopentane, 1-pentyl-2-propyl-    46122 062199-51-3 60

25  12.048  1.61 C:\Database\NIST08.L
                Bicyclo[3.1.1]heptane, 2,6,6-trime  16802 006876-13-7 64
                thyl-, (1.alpha.,2.beta.,5.alpha.)
                Bicyclo[3.1.1]heptane, 2,6,6-trime  16765 000473-55-2 52
                thyl-
                Bicyclo[3.1.1]heptane, 2,6,6-trime  16805 004795-86-2 46
                thyl-, [1R-(1.alpha.,2.beta.,5.alp
                ha.)]-

26  12.177  0.35 C:\Database\NIST08.L
                Cyclohexanol, 1-ethynyl-            10389 000078-27-3 38
                Cyclohexanol, 1-ethynyl-            10387 000078-27-3 38
                3,7,11,15-Tetramethyl-2-hexadecen- 133816 102608-53-7 35
                1-ol

27  12.281  0.54 C:\Database\NIST08.L
                3,7,11,15-Tetramethyl-2-hexadecen- 133816 102608-53-7 53
                1-ol
                Cyclohexanol, 1-ethynyl-            10387 000078-27-3 50
                Cyclohexanol, 1-ethynyl-            10389 000078-27-3 50

28  12.455 20.13 C:\Database\NIST08.L
                Caffeine                            55116 000058-08-2 97
                Caffeine                            55118 000058-08-2 97
                Caffeine                            55120 000058-08-2 97

29  12.656  0.66 C:\Database\NIST08.L
                Purine-2,6(1H,3H)-dione, 1-(2-ethe  97335 1000272-53-5 91
                nyloxyethyl)-3,7-dimethyl-
                Theobromine                         44941 000083-67-0 83
                Theobromine                         44939 000083-67-0 80

30  12.805  0.72 C:\Database\NIST08.L
                n-Hexadecanoic acid                102726 000057-10-3 99
                n-Hexadecanoic acid                102725 000057-10-3 98
                n-Hexadecanoic acid                102724 000057-10-3 96

31  12.863  0.43 C:\Database\NIST08.L
                Hexadecanoic acid, ethyl ester     124589 000628-97-7 95
                Hexadecanoic acid, ethyl ester     124591 000628-97-7 93
                Ethyl tridecanoate                  91831 028267-29-0 72

32  12.934  0.13 C:\Database\NIST08.L
                Tricyclo[4.2.1.1(2,5)]decan-9-ol,   24830 066953-30-8 11
                stereoisomer
                Tricyclo[5.2.1.0(4,8)]decan-5-ol    24734 1000190-98-9 10
                1,5:2,4-Dimethanopentalene-3,6-dio  34182 066486-73-5 10
                l, octahydro-

33  13.277  0.05 C:\Database\NIST08.L
                Octadecanoic acid, 2-propenyl este 154534 006289-31-2 32
                2,6-Heptadienoic acid, 3-methyl-,   27229 062185-61-9 18
                methyl ester
                Furan, tetrahydro-2,2,5,5-tetramet  12506 015045-43-9 14
                hyl-

34  13.329  0.03 C:\Database\NIST08.L
                Cyclotrisiloxane, hexamethyl-       76687 000541-05-9 43
                8-Morpholino-4-cycloocten-1-one ox  77763 1000240-66-4 38
                ime
                Phenanthridinium, 5,6-dimethyl-, i 162050 016511-48-1 27
                odide
```

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35  13.413  0.03 C:\Database\NIST08.L
             Benzaldehyde, 3-ethoxy-2-hydroxy-   34950 000492-88-6 25
             E-11(13,13-Dimethyl)tetradecen-1-o 122841 1000130-80-2 14
             l acetate
             Pregn-4-ene-3,20-dione, 6,16-dimet 167012 001816-79-1 12
             hyl-, (6.beta.,16.alpha.)-

36  13.710  3.00 C:\Database\NIST08.L
             Octadec-9-enoic acid               122782 1000190-13-7 99
             cis-Vaccenic acid                  122781 000506-17-2 96
             cis-13-Octadecenoic acid           122788 013126-39-1 96

37  13.833  1.32 C:\Database\NIST08.L
             Octadecanoic acid, ethyl ester     145977 000111-61-5 91
             Octadecanoic acid, ethyl ester     145980 000111-61-5 72
             Methyl 17-methyl-octadecanoate     145986 1000336-21-8 72

38  14.027  0.33 C:\Database\NIST08.L
             Hexestrol di-TMS                   199748 070244-15-4 43
             7-Chloro-4-methoxy-3-methylquinoli  64522 1000213-52-2 38
             ne
             5,5'-Di(ethoxycarbonyl)-3,3'-dimet 196389 102586-97-0 37
             hyl-4,4'-dipropyl-2,2'-dipyrrylmet
             hane

39  14.124  0.37 C:\Database\NIST08.L
             1-Hexyl-2-nitrocyclohexane          69413 118252-04-3 80
             i-Propyl 11-octadecenoate          154529 1000336-79-5 80
             Cyclododecanemethanol               58023 001892-12-2 72

40  14.195  0.17 C:\Database\NIST08.L
             Octanamide, N,N-dimethyl-           38130 001118-92-9 59
             6-(2-Acetoxyethoxy)-4-nitrobenzofu 123084 293324-91-1 47
             roxan
             Acetohydrazide, 2-(2-methyl-1,3-di 155279 1000258-56-8 47
             oxolan-2-yl)-N2-(4-bromobenzyliden
             o)-

41  14.228  0.13 C:\Database\NIST08.L
             7-Hydroxy-2,4,6-trimethyl-8-oxazol 121802 104418-91-9 16
             -5-yloct-2-enoic acid, methyl este
             Benzenamine, 4-nitroso-N-phenyl-    57712 000156-10-5  9
             Phosphine, dicyclohexyl-            57904 000829-84-5  9

42  14.280  0.30 C:\Database\NIST08.L
             3-Cyclopentylpropionic acid, 2-dim  69420 1000331-24-3 78
             ethylaminoethyl ester
             Octanoic acid, 2-dimethylaminoethy  70878 1000330-94-6 78
             l ester
             Ethanamine, 2-[4-(1,2-diphenyl-1-b 183511 010540-29-1 53
             utenyl)phenoxy]-N,N-dimethyl-, (Z)

43  14.370  0.32 C:\Database\NIST08.L
             1H-Tetrazole-1-ethanol, 5-amino-    12635 015284-29-4 35
             Piperidine, 1-(ethoxymethyl)-       20061 003275-13-6 15
             Cyclopentanone, 2-ethyl-             6479 004971-18-0 11

44  14.499  0.30 C:\Database\NIST08.L
             16-Octadecenal                     110392 056554-87-1 64
             Tridecane, 7-cyclohexyl-           110450 013151-92-3 50
             1,19-Eicosadiene                   119881 014811-95-1 45

45  14.538  0.19 C:\Database\NIST08.L
             5-Amino-2-(4-chlorophenyl)-7-methy 121829 1000305-54-5 38
             l-6-indolizinecarbonitrile
             9-Phenanthrenemethyl 3,4,5-trimeth 196439 092206-04-7 22
             oxybenzoate
             7,9-Dimethyl-7H-5,6,7,9,11a-pentaa 121654 1000301-21-2 15
             za-benzo[a]fluorene-8,10-dione
```

46	14.655	0.25	C:\Database\NIST08.L			
			Benzeneacetaldehyde, .alpha.-(phen ylmethylene)-	65694	013702-35-7	18
			Benzene, 1-methyl-2-(phenylmethyl)	46166	000713-36-0	15
			Bendazol	65564	000621-72-7	14
47	14.784	0.18	C:\Database\NIST08.L			
			Benzo[h]quinoline, 2,4-dimethyl-	64840	000605-67-4	41
			Trimethyl(4-tert.-butylphenoxy)sil ane	76225	025237-79-0	35
			1H-Indole, 1-methyl-2-phenyl-	64833	003558-24-5	35
48	14.888	0.14	C:\Database\NIST08.L			
			2-(5-Adamantan-1-yl-[1,2,4]oxadiaz ol-3-yl)-pyridine	121922	1000310-56-9	11
			1,3-Dihydroxy-2,4,5-trifluoro-6-ni trobenzene	66461	031438-88-7	11
			7-Chloro-4-methylquinoline-2-thiol	66189	1000303-46-7	10
49	14.920	0.08	C:\Database\NIST08.L			
			Phenol, 2,6-dimethyl-4-nitro-	35359	002423-71-4	25
			1,3-Benzodioxole, 5-nitro-	35251	002620-44-2	22
			[1,2,3]Triazolo[4,5-e][1,4]diazepi ne-5,8-dione, 1,4,6,7-tetrahydro-	35218	1000142-39-0	22
50	14.998	0.27	C:\Database\NIST08.L			
			9,12-Octadecadien-1-ol, (Z,Z)-	110413	000506-43-4	80
			Z,Z-3,13-Octadecadien-1-ol	110410	1000131-10-9	72
			9-Octadecenal, (Z)-	110397	002423-10-1	55
51	15.049	0.40	C:\Database\NIST08.L			
			9-Octadecenamide, N,N-dimethyl-	143537	003906-30-7	93
			Non-7-enoic acid, dimethylamide	46756	1000187-26-5	50
			Octanamide, N,N-dimethyl-	38125	001118-92-9	47
52	15.120	0.39	C:\Database\NIST08.L			
			O-[n-Propylcarbamoyl]-3-exo-dimeth ylaminomethyl-2-norbornanone oxime	110847	1000211-95-3	59
			DL-Norepinephrine, N,N-dimethyl-, trimethyl ether	89223	1000332-93-6	45
			Amitryptyline	119043	000050-48-6	45
53	15.237	0.65	C:\Database\NIST08.L			
			Cyclohexanecarboxylic acid, decyl ester	111923	093479-48-2	38
			9-Octadecenoic acid (Z)-, 2-hydrox y-1-(hydroxymethyl)ethyl ester	175175	003443-84-3	25
			Cyclohexanecarboxylic acid, tetrad ecyl ester	154542	1000279-54-2	22
54	15.373	0.26	C:\Database\NIST08.L			
			.gamma.-Cyano-3-methyl-5,10-dihydr obenzo[f]indolizine	65603	1000213-00-8	50
			3-Phenyl-2H-chromene	65665	006054-00-8	50
			Cyclohexane-1,3-dione, 2-allylamin omethylene-5,5-dimethyl-	64744	104926-37-6	35
55	15.431	0.11	C:\Database\NIST08.L			
			Quinoline, 3-bromo-	64962	005332-24-1	30
			3-Bromo-2-([[(3-bromothien-2-yl)th io]methyl]thio)thiophene	195962	1000305-68-2	27
			9-Borabicyclo[3.3.1]nonane, 9-[3-(dimethylamino)propyl]-	64801	1000160-35-2	11
56	15.528	0.52	C:\Database\NIST08.L			
			Stannane, tetrakis(1-methylethyl)-	130116	002949-42-0	83
			3-Phenyl-2H-chromene	65665	006054-00-8	30
			2,3,4-Trimethoxyphenylacetonitrile	64550	068913-85-9	15

57	15.644	0.28	C:\Database\NIST08.L			
			Anthracene, 9,10-dihydro-9,9,10-tr imethyl-	76655	014923-29-6	43
			1,2-Bis(trimethylsilyl)benzene	76049	017151-09-6	38
			Chlorodibromoacetic acid, methyl e ster	108952	020428-75-5	38
58	15.716	0.17	C:\Database\NIST08.L			
			2-Ethylacridine	64819	055751-83-2	43
			Anthracene, 9-ethyl-9,10-dihydro-1 0-t-butyl-	108946	1000154-57-7	43
			2-Amino-4-hydroxy-6,8-dimethyl-7(8 H)-pteridinone	64928	025477-64-9	43
59	15.806	0.27	C:\Database\NIST08.L			
			2-(Acetoxymethyl)-3-(methoxycarbon yl)biphenylene	122638	093103-70-9	53
			5-Methyl-2-trimethylsilyloxy-aceto phenone	76038	097389-69-0	47
			Propiophenone, 2'-(trimethylsiloxy)-	76035	033342-87-9	47
60	15.832	0.17	C:\Database\NIST08.L			
			Terephthalaldehydic acid, methyl e ster, p-(O-methyloxime)	53699	033499-35-3	35
			Benzonitrile, 3,5-dinitro-	54014	004110-35-4	16
			Pyridin-4-amine, 2,3-dichloro-	31789	184416-83-9	14
61	15.890	0.06	C:\Database\NIST08.L			
			9H-Fluorene-4-carboxylic acid, 9-o xo-, (2,6-dimethylphenyl)amide	156670	1000304-78-2	38
			5,5'-Di(ethoxycarbonyl)-3,3'-dimet hyl-4,4'-dipropyl-2,2'-dipyrrylmet hane	196389	102586-97-0	28
			1-(4-Chloro-phenyl)-5-[4-(1,1,2,2- tetrafluoro-ethoxy)-benzylsulfanyl]-1H-tetrazole	200623	1000275-06-7	25
62	15.916	0.10	C:\Database\NIST08.L			
			No matches found			
63	15.955	0.14	C:\Database\NIST08.L			
			Silane, 1,4-phenylenebis[trimethyl	76051	013183-70-5	53
			1-Propene, 3-(2-cyclopentenyl)-2-m ethyl-1,1-diphenyl-	116987	1000154-23-3	52
			N-Methyl-1-adamantaneacetamide	64771	031897-93-5	52
64	16.007	0.13	C:\Database\NIST08.L			
			Pyridine, 1,2,3,6-tetrahydro-1-met hyl-4-[4-chlorophenyl]-	64646	005048-08-8	49
			2-(Acetoxymethyl)-3-(methoxycarbon yl)biphenylene	122638	093103-70-9	35
			Bendazol	65564	000621-72-7	27
65	16.033	0.21	C:\Database\NIST08.L			
			Acethydrazide, N2-[1-(2-hydroxyphe nyl)ethylidene]-2,2-diphenyl-	168190	314764-55-1	32
			2,2-Diphenylethylamine	57179	003963-62-0	27
			Succinic acid, eicosyl 2-methylpen t-3-yl ester	211644	1000349-39-9	9
66	16.110	0.16	C:\Database\NIST08.L			
			N-Methyl-1-adamantaneacetamide	64771	031897-93-5	25
			Benzene, 1,3,5-trichloro-2-(1-meth ylethyl)-	76884	054965-70-7	25
			Benzene, 1-(1,1-dimethylethyl)-4-(2-ethoxyethoxy)-	76317	054889-97-3	25
67	16.149	0.08	C:\Database\NIST08.L			
			Dibenzo[b,E]-8-azabicyclo[3,2,1]oc	142785	1000129-09-9	50

			tane, N-[N-[3-hydroxypropyl]aminoc arbonyl]-			
			4-Ethylacridine	64818	065789-44-8	50
			Benzene, 1,1'-(1-cyclobutene-1,2-d iyl)bis-	64172	003306-02-3	30
68	16.181	0.13	C:\Database\NIST08.L			
			Sarcosine, N-(2-methylbenzoyl)-, h exadecyl ester	203876	1000321-17-6	22
			Pyrazol-2(5H)-one, 5-(4-fluorophen yl)-3-hydroxy-4-(4-methylbenzoyl)- 1-(3-pyridinylmethyl)-	196406	1000273-91-0	22
			1-Benzothiazol-2-yl-3-(4-methyl-be nzoyl)-thiourea	156294	131120-12-2	22
69	16.227	0.14	C:\Database\NIST08.L			
			Acrylonitrile, 3-bicyclo[2.2.1]hep t-5-en-2-yl-2-(5-methyl-1H-benzoim idazol-2-yl)-	117572	1000309-94-2	27
			2-Propen-1-one, 1,3-diphenyl-	65684	000094-41-7	25
			Benzene, 1,1'-(1,2-dimethyl-1,2-et henediyl)bis-, (Z)-	65778	000782-05-8	18
70	16.324	0.29	C:\Database\NIST08.L			
			2-Butenenitrile, 2-chloro-3-(4-met hoxyphenyl)-	64528	1000305-66-7	25
			Cyclobarbital	86685	000052-31-3	22
			1H-1,3-Benzimidazole-1-acetonitril e, 2-(difluoromethyl)-	64484	1000351-67-7	22
71	16.434	0.50	C:\Database\NIST08.L			
			Heneicosane, 3-methyl-	144476	006418-47-9	10
			Tetrahydrofuran-2-carboxylic acid, dibenzofuran-3-ylamide	121907	1000316-12-2	9
			2-Amino-N-[2-((1-[4-amino-6-(dimet hylamino)-1,3,5-triazin-2-yl]-2-ph enylethyl)amino)-1-benzyl-2-oxoeth yl]-3-phenylpropanamide	216293	057227-01-7	8
72	16.505	0.20	C:\Database\NIST08.L			
			1H-Pyrazole-5-carboxylic acid, 3-[[(4-bromophenyl)amino]carbonyl]-1- methyl-, methyl ester	163118	1000350-46-3	9
			2,2-Diphenylethylamine	57179	003963-62-0	4
			2,2-Diphenylethylamine	57181	003963-62-0	4
73	16.589	0.13	C:\Database\NIST08.L			
			Indole, 2,3-dihydro-3-[2-[N-(2-men thyloxycarbonyl)-N-methylamino]eth yl]	200299	1000124-26-9	2
74	17.262	0.31	C:\Database\NIST08.L			
			2,6-Octadiene, 2,7-dimethyl-	16698	016736-42-8	64
			Squalene	198698	007683-64-9	64
			2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	198716	000111-02-4	64
75	18.232	0.01	C:\Database\NIST08.L			
			No matches found			
76	18.271	0.01	C:\Database\NIST08.L			
			Antra-9,10-quinone, 1-(3-hydrohy-3 -phenyl-1-triazenyl)-	167418	098496-82-3	47
			Silicic acid, diethyl bis(trimethy lsilyl) ester	132967	003555-45-1	38
			1-Propene, 3-(2-cyclopentenyl)-2-m ethyl-1,1-diphenyl-	116987	1000154-23-3	38

```
File       :C:\msdchem\CAL 2010\DATA\2014\Yaakob\CAL-06.D
Operator   : Hasbullah
Acquired   : 12 Jul 2014  13:08     using AcqMethod BOIL-001NORIZAN.M
Instrument :   gcms1
Sample Name: OOE
Misc Info  :
Vial Number: 1
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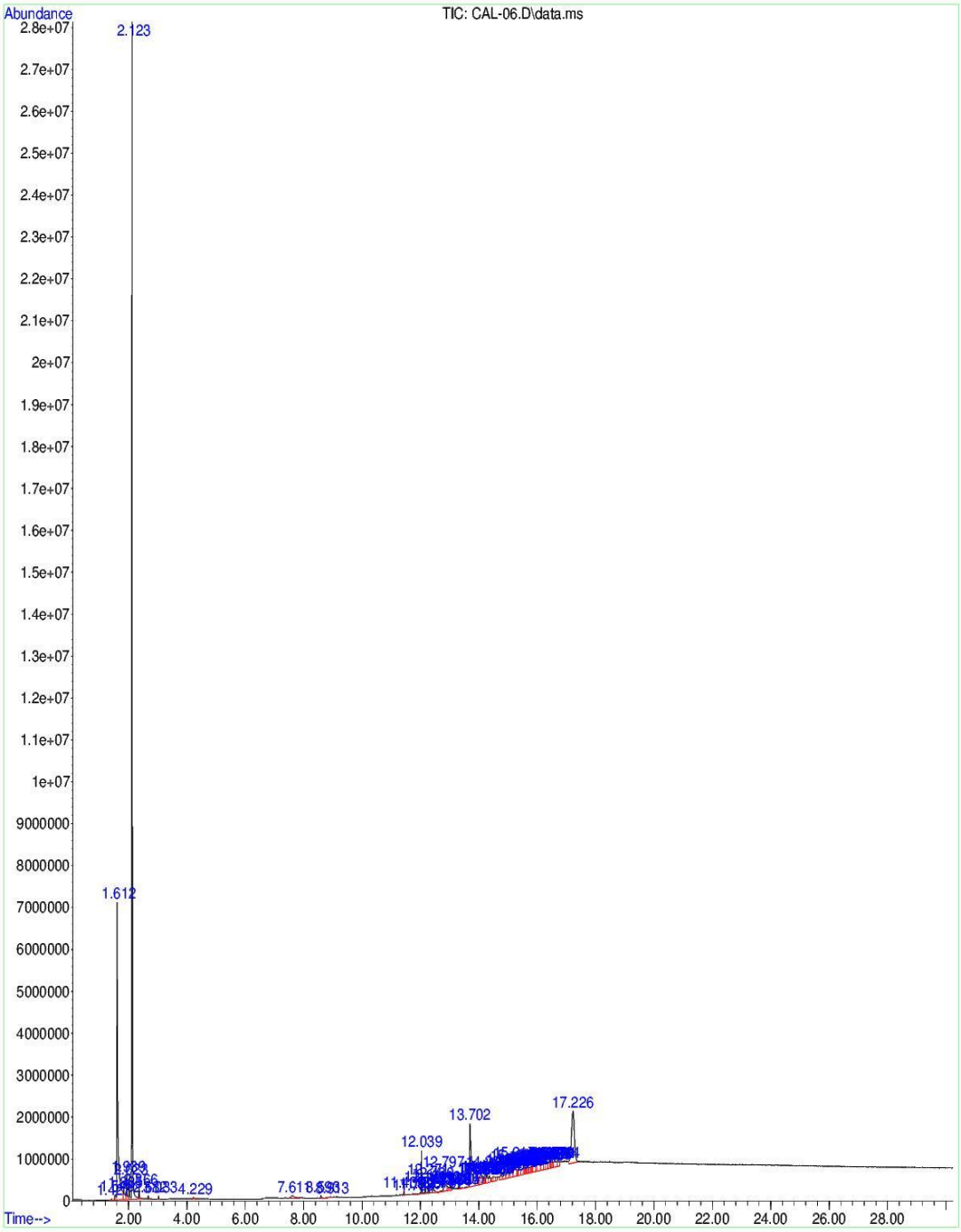


Area Percent Report

Acq On : 12 Jul 2014 13:08

Sample : OOE
Data File : CAL-06.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Integration Parameters: genie.e

Signal : TIC: CAL-06.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.427	195	207	211	PV	35012	381592	0.11%	0.039%
2	1.543	211	225	232	PV	120730	3773489	1.13%	0.385%
3	1.612	232	236	267	VV	6661523	150735583	45.33%	15.387%
4	1.835	267	270	282	VV 3	204485	7794596	2.34%	0.796%
5	1.939	282	286	295	VV	560216	9481291	2.85%	0.968%
6	2.023	295	299	309	VV	455610	7333134	2.21%	0.749%
7	2.123	309	315	345	VV	26913382	332513720	100.00%	33.943%
8	2.366	349	352	375	VV	246264	3963960	1.19%	0.405%
9	2.682	397	401	412	PV	74538	1094918	0.33%	0.112%
10	3.033	450	455	462	PB	82185	936242	0.28%	0.096%
11	4.229	632	640	662	PV 3	37346	962509	0.29%	0.098%
12	7.611	1150	1163	1200	VV 5	62569	4856497	1.46%	0.496%
13	8.593	1311	1315	1329	VV 2	66259	1500774	0.45%	0.153%
14	8.913	1334	1364	1367	BV 2	4463	202880	0.06%	0.021%
15	11.435	1747	1754	1761	VV 2	91426	1364365	0.41%	0.139%
16	11.753	1790	1803	1810	PV 2	19859	607067	0.18%	0.062%
17	11.996	1826	1841	1843	PV 9	31532	493291	0.15%	0.050%
18	12.039	1843	1848	1862	VV	968509	12071869	3.63%	1.232%
19	12.169	1862	1868	1874	VV 2	178971	2362659	0.71%	0.241%
20	12.271	1879	1884	1889	VV	328853	3816615	1.15%	0.390%
21	12.430	1897	1908	1920	VV	262745	6320259	1.90%	0.645%
22	12.513	1920	1921	1932	VV	23856	601434	0.18%	0.061%
23	12.711	1932	1952	1954	PV	21792	727656	0.22%	0.074%
24	12.741	1954	1956	1958	VV 3	11760	128059	0.04%	0.013%
25	12.797	1958	1965	1983	VV	466372	18410406	5.54%	1.879%
26	12.925	1983	1985	1991	VV 6	112010	2980916	0.90%	0.304%
27	12.989	1991	1994	2003	VV 6	75599	3085116	0.93%	0.315%
28	13.055	2003	2005	2009	VV 5	46645	923912	0.28%	0.094%
29	13.295	2034	2042	2044	VV 5	38930	1007450	0.30%	0.103%
30	13.324	2044	2046	2053	VV 8	31154	639483	0.19%	0.065%
31	13.407	2053	2059	2061	VV 7	30005	571460	0.17%	0.058%
32	13.577	2070	2085	2090	PV 7	22870	660536	0.20%	0.067%
33	13.702	2090	2105	2148	PV 2	1471759	89201837	26.83%	9.106%
34	13.988	2148	2149	2151	VV 2	187103	2644249	0.80%	0.270%
35	14.015	2151	2153	2163	VV 10	183743	7567285	2.28%	0.772%
36	14.114	2163	2168	2170	VV 6	205108	4750813	1.43%	0.485%
37	14.131	2170	2171	2176	VV 5	197733	3840669	1.16%	0.392%
38	14.182	2176	2179	2183	VV 4	153208	3345629	1.01%	0.342%
39	14.220	2183	2185	2188	VV 4	121496	2414319	0.73%	0.246%
40	14.268	2188	2192	2199	VV	278369	6616516	1.99%	0.675%
41	14.356	2199	2206	2213	VV 8	159132	5994616	1.80%	0.612%
42	14.469	2218	2223	2225	VV 6	100855	2795366	0.84%	0.285%
43	14.509	2225	2229	2241	VV 6	114929	5566082	1.67%	0.568%

44	14.607	2241	2245	2247	VV	4	87348	2102617	0.63%	0.215%
45	14.754	2259	2267	2276	VV	4	108921	5355396	1.61%	0.547%
46	14.866	2276	2285	2293	VV	4	119477	5935425	1.79%	0.606%
47	14.980	2293	2302	2307	VV	2	231716	7712091	2.32%	0.787%
48	15.028	2307	2310	2315	VV	5	141159	3779404	1.14%	0.386%
49	15.104	2315	2322	2331	VV		309336	12965387	3.90%	1.323%
50	15.217	2331	2339	2351	VV	5	359894	15238676	4.58%	1.556%
51	15.300	2351	2352	2354	VV	2	137213	1595471	0.48%	0.163%
52	15.336	2354	2357	2360	VV	5	144188	3726105	1.12%	0.380%
53	15.382	2360	2364	2372	VV	10	149436	6184844	1.86%	0.631%
54	15.491	2372	2381	2387	VV	10	143832	7747504	2.33%	0.791%
55	15.538	2387	2389	2392	VV	4	137504	2890918	0.87%	0.295%
56	15.577	2392	2395	2396	VV	3	139514	1800411	0.54%	0.184%
57	15.599	2396	2398	2403	VV	6	141073	3475161	1.05%	0.355%
58	15.641	2403	2405	2406	VV	2	142118	1966549	0.59%	0.201%
59	15.682	2406	2411	2413	VV	6	137949	3348599	1.01%	0.342%
60	15.707	2413	2415	2416	VV	2	134908	1864832	0.56%	0.190%
61	15.765	2416	2424	2425	VV	9	141058	4396134	1.32%	0.449%
62	15.785	2425	2427	2431	VV	5	142111	3166315	0.95%	0.323%
63	15.824	2431	2433	2435	VV	3	144186	2409176	0.72%	0.246%
64	15.894	2435	2444	2449	VV	3	149312	7461124	2.24%	0.762%
65	15.964	2449	2454	2456	VV	6	148265	3919635	1.18%	0.400%
66	16.111	2456	2477	2478	VV	6	150104	12254681	3.69%	1.251%
67	16.170	2478	2486	2493	VV	6	155051	8825290	2.65%	0.901%
68	16.228	2493	2495	2501	VV	7	150548	4189416	1.26%	0.428%
69	16.347	2501	2514	2515	VV	7	151204	8214606	2.47%	0.839%
70	16.374	2515	2518	2524	VV	8	157440	5314329	1.60%	0.542%
71	16.428	2524	2526	2530	VV	4	145689	2983727	0.90%	0.305%
72	16.466	2530	2532	2533	VV	2	137510	1890070	0.57%	0.193%
73	16.519	2533	2540	2542	VV	7	137317	4399068	1.32%	0.449%
74	16.542	2542	2544	2546	VV	3	135712	1968691	0.59%	0.201%
75	16.631	2546	2557	2566	VV	3	132718	9925441	2.98%	1.013%
76	16.744	2566	2575	2579	VV	3	113732	5465685	1.64%	0.558%
77	17.226	2626	2650	2677	VV	2	1237199	88115028	26.50%	8.995%

Sum of corrected areas: 979628924

B-OIL.M Wed Jul 16 09:39:30 2014

Library Search Report

Acq On : 12 Jul 2014 13:08

Sample : OOE
Data File : CAL-06.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Search Libraries: C:\Database\NIST08.L Minimum Quality: 50

Unknown Spectrum: Apex minus start of peak
Integration Events: ChemStation Integrator - genie.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.426	0.04	C:\Database\NIST08.L			
			Acetaldehyde	71	000075-07-0	2
			Butanoic acid, 2-oxo-	4197	000600-18-0	2
			Ethylene oxide	74	000075-21-8	2
2	1.543	0.39	C:\Database\NIST08.L			
			Adenosine, 2-methyl-	121459	016526-56-0	3
			Methyl formate	265	000107-31-3	2
			Methylamine	28	000074-89-5	2
3	1.614	15.39	C:\Database\NIST08.L			
			Ethanol	95	000064-17-5	90
			Ethanol	94	000064-17-5	86
			Ethanol	93	000064-17-5	78
4	1.834	0.80	C:\Database\NIST08.L			
			Methylene Chloride	1517	000075-09-2	93
			Methylene Chloride	1516	000075-09-2	90
			Methylene Chloride	1519	000075-09-2	87
5	1.937	0.97	C:\Database\NIST08.L			
			Pentane, 2-methyl-	1816	000107-83-5	91
			Pentane, 2-methyl-	1814	000107-83-5	91
			Butane, 2,3-dimethyl-	1819	000079-29-8	59
6	2.021	0.75	C:\Database\NIST08.L			
			Pentane, 3-methyl-	1817	000096-14-0	91
			Pentane, 3-methyl-	1815	000096-14-0	91
			Pentane, 3-methyl-	1818	000096-14-0	91
7	2.125	33.94	C:\Database\NIST08.L			
			Hexane	1812	000110-54-3	94
			Hexane	1813	000110-54-3	64
			Hexane	1811	000110-54-3	59
8	2.364	0.40	C:\Database\NIST08.L			
			Cyclohexane	1452	000110-82-7	83
			Cyclobutane, ethyl-	1464	004806-61-5	64
			1H-Tetrazole, 5-methyl-	1323	004076-36-2	64
9	2.681	0.11	C:\Database\NIST08.L			
			Cyclohexane	1450	000110-82-7	74
			Cyclohexane	1451	000110-82-7	74
			1-Hexene	1447	000592-41-6	64
10	3.031	0.10	C:\Database\NIST08.L			
			Heptane	3942	000142-82-5	95
			Heptane	3941	000142-82-5	91
			Heptane	3940	000142-82-5	91
11	4.227	0.10	C:\Database\NIST08.L			
			Oxalic acid, isohexyl pentyl ester	92962	1000309-32-8	64

			Sulfurous acid, hexyl pentadecyl e ster	185908	1000309-13-7	59
			Oxalic acid, dodecyl isohexyl este	166793	1000309-33-5	59
12	7.610	0.50	C:\Database\NIST08.L			
			3,4-Dimethyl-3-pyrrolin-2-one	6067	004030-22-2	78
			Pyrimidine, 4-hydroxy-	2706	051953-18-5	38
			1H-Imidazole, 1,4-dimethyl-	2743	006338-45-0	38
13	8.594	0.15	C:\Database\NIST08.L			
			3-Tridecene, (E)-	46103	041446-57-5	43
			Cyclopentane, 1,2,3-trimethyl-, (1 .alpha.,2.alpha.,3.alpha.)-	6770	002613-69-6	38
			Cyclopentane, 1,2,3-trimethyl-, (1 .alpha.,2.alpha.,3.alpha.)-	6772	002613-69-6	38
14	8.911	0.02	C:\Database\NIST08.L			
			Benzofuran, 2,3-dihydro-	9282	000496-16-2	64
			N-Phthaloyltyramine	110961	064985-42-8	53
			Benzocaine	33862	000094-09-7	52
15	11.433	0.14	C:\Database\NIST08.L			
			1-Hexadecanol, 2-methyl-	102837	002490-48-4	86
			1-Undecene, 8-methyl-	35974	074630-40-3	81
			3-Tetradecene, (Z)-	56572	041446-67-7	68
16	11.750	0.06	C:\Database\NIST08.L			
			Cyclohexane, 1,2,3-trimethyl-	11467	001678-97-3	41
			7-Tetradecene	56563	010374-74-0	35
			Bicyclo[3.1.1]heptan-3-one, 2-ethy 1-6,6-dimethyl-	34368	1000163-95-8	30
17	11.996	0.05	C:\Database\NIST08.L			
			Cyclohexane, 2-butyl-1,1,3-trimeth yl-	46129	054676-39-0	58
			3-Undecene, 9-methyl-, (E)-	36030	074630-54-9	41
			4-Undecene, 9-methyl-, (Z)-	36035	074630-56-1	38
18	12.041	1.23	C:\Database\NIST08.L			
			Bicyclo[3.1.1]heptane, 2,6,6-trime thyl-, (1.alpha.,2.beta.,5.alpha.)	16802	006876-13-7	58
			Bicyclo[3.1.1]heptane, 2,6,6-trime thyl-	16765	000473-55-2	52
			Bicyclo[3.1.1]heptane, 2,6,6-trime thyl-	16757	000473-55-2	49
19	12.171	0.24	C:\Database\NIST08.L			
			3,7,11,15-Tetramethyl-2-hexadecen- 1-ol	133816	102608-53-7	59
			Cyclohexane, 1-methyl-4-(1-methyle thenyl)-, trans-	16797	001124-25-0	49
			Cyclohexanol, 1-ethynyl-	10389	000078-27-3	47
20	12.274	0.39	C:\Database\NIST08.L			
			1,4-Eicosadiene	119879	1000131-16-3	80
			Dodeca-1,6-dien-12-ol, 6,10-dimeth yl-	67173	1000156-13-8	64
			Cyclohexanol, 1-ethynyl-	10387	000078-27-3	50
21	12.429	0.65	C:\Database\NIST08.L			
			Caffeine	55116	000058-08-2	97
			Caffeine	55119	000058-08-2	97
			Caffeine	55120	000058-08-2	96
22	12.514	0.06	C:\Database\NIST08.L			
			1H-1,2,4-Triazole-5(4H)-thione, 4- allyl-3-(3-furyl)-	64981	1000277-38-2	22
			2,3,4-Trimethoxyphenylacetonitrile	64550	068913-85-9	18
			Anthracene, 9,10-dihydro-9,9,10-tr imethyl-	76655	014923-29-6	14

23	12.714	0.07	C:\Database\NIST08.L			
			Benzene-1,3-dicarboxylic acid, 5-h ydroxymethyl-, diethyl ester	99048	181425-91-2	38
			Benzo[h]quinoline, 2,4-dimethyl-	64841	000605-67-4	27
			1H-Indole, 5-methyl-2-phenyl-	64835	013228-36-9	27
24	12.740	0.01	C:\Database\NIST08.L			
			7-Chlorocinchoninic acid	64463	013337-66-1	46
			3-Amino-7-nitro-1,2,4-benzotriazin e 1-oxide	64885	1000256-54-1	43
			Quinoline, 3-bromo-	64962	005332-24-1	37
25	12.798	1.88	C:\Database\NIST08.L			
			n-Hexadecanoic acid	102726	000057-10-3	99
			n-Hexadecanoic acid	102725	000057-10-3	98
			n-Hexadecanoic acid	102724	000057-10-3	98
26	12.928	0.30	C:\Database\NIST08.L			
			Isocyanate, 4-pyridinyl	9224	1000337-70-6	9
			1,2,4,3,5-Triselenadiborolane, 3,5 -diethyl-	151955	115706-03-1	9
			Furan-2-carboxamide, N-(2,4-dimeth oxyphenyl)-	95358	328258-35-1	8
27	12.986	0.31	C:\Database\NIST08.L			
			1H-Indole, 3-methyl-2-(2'-pyridyl)	65587	000951-25-7	38
			Xanthine, 1,3,7,8-tetramethyl-	65984	000832-66-6	37
			Xanthine, 1,3,7,8-tetramethyl-	65983	000832-66-6	37
28	13.057	0.09	C:\Database\NIST08.L			
			1-(5'-Chloro-2'-methylaminobenzoyl)-cyclohex-1-ene	96915	097994-57-5	30
			1,2-Dimethyl-4-azaphenanthrene-3-c arboxylic acid	98629	1000298-84-6	16
			1H-Indole, 1-methyl-2-phenyl-	64833	003558-24-5	14
29	13.296	0.10	C:\Database\NIST08.L			
			2,6-Octadien-1-ol, 3,7-dimethyl-, acetate	56315	016409-44-2	27
			2,5,9,13-Tetramethyl-tetradeca-4,8 ,12-trienoic acid, methyl ester	130801	055844-49-0	16
			2-Dodecene, 2-methyl-	46117	055103-82-7	14
30	13.322	0.07	C:\Database\NIST08.L			
			1H-Indole, 5-methyl-2-phenyl-	64835	013228-36-9	43
			Benzo[h]quinoline, 2,4-dimethyl-	64841	000605-67-4	38
			2-Ethylacridine	64819	055751-83-2	38
31	13.406	0.06	C:\Database\NIST08.L			
			Orthocaine acetate	66110	1000120-03-6	11
			Pyridine-3-carboxamide, oxime, N-(2-trifluoromethylphenyl)-	121557	288246-53-7	10
			Methyl Z-11-tetradecenoate	90217	1000130-82-8	10
32	13.574	0.07	C:\Database\NIST08.L			
			4-Nonene, 5-butyl-	46114	007367-38-6	35
			Cyclohexanecarboxamide, N-furfuryl	64671	006341-32-8	35
			Fumaric acid, 2,5-dichlorophenyl d odecyl ester	203111	1000345-32-5	25
33	13.704	9.11	C:\Database\NIST08.L			
			cis-Vaccenic acid	122781	000506-17-2	99
			cis-13-Octadecenoic acid	122788	013126-39-1	96
			trans-13-Octadecenoic acid	122798	000693-71-0	95
34	13.988	0.27	C:\Database\NIST08.L			
			Brallobarbital	125417	000561-86-4	35
			4-Quinolinecarboxylic acid, 2-chlo ro-	64470	005467-57-2	30

			3-Amino-7-nitro-1,2,4-benzotriazin e 1-oxide	64885	1000256-54-1	27
35	14.014	0.77	C:\Database\NIST08.L			
			1-Cyclopropyl-6,7,8-trifluoro-4-ox o-1,4-dihydroquinoline-3-carboxyli c acid, ethyl ester	144704	094242-51-0	10
			Carbonic acid, monoamide, N-(5-chl oro-2-methoxyphenyl)-, propargyl e ster	89053	1000340-17-6	10
			Benzeneacetic acid, .alpha.-hydrox y-.alpha.-phenyl-, 1-methyl-4-pipe ridinyl ester	155117	003608-67-1	10
36	14.111	0.48	C:\Database\NIST08.L			
			1-Hexyl-1-nitrocyclohexane	69414	118252-09-8	52
			1-Hexyl-2-nitrocyclohexane	69413	118252-04-3	52
			Cyclopentanecarboxylic acid, 2-tri decyl ester	133740	1000280-58-4	47
37	14.131	0.39	C:\Database\NIST08.L			
			9-Borabicyclo[3.3.1]nonane, 9-[3-(dimethylamino)propyl]-	64801	1000160-35-2	38
			Propanenitrile, 3-(5-diethylamino- 1-methyl-3-pentynyloxy)-	76213	016454-78-7	35
			Indolo[2,3-b]quinolizine, 1,2,3,4, 6,7,12,12b-octahydro-12-methyl-	90379	013233-45-9	11
38	14.182	0.34	C:\Database\NIST08.L			
			(2-Methyl-[1,3]dioxolan-2-yl)-acet ic acid, phenyl ester	75994	1000189-52-7	53
			Octanamide, N,N-dimethyl-	38130	001118-92-9	46
			Thiocyanic acid, ethyl ester	1844	000542-90-5	38
39	14.221	0.25	C:\Database\NIST08.L			
			Quinolin-2-ol, 6-chloro-4-methyl-O -[5-[1-cycloazapropyl]-n-pentyl]-	139662	041288-78-2	22
			Phenol, 4-[2-[2-(chloromethyl)-1,3 -dioxolan-2-yl]ethyl]-, acetate	123966	055255-66-8	16
			2H-1,4-Benzoxazine-6-carboxylic ac id, 3,4-dihydro-3-oxo-	54128	1000351-35-0	10
40	14.267	0.68	C:\Database\NIST08.L			
			Octanoic acid, 2-dimethylaminoethy l ester	70878	1000330-94-6	72
			3-Cyclopentylpropionic acid, 2-dim ethylaminoethyl ester	69420	1000331-24-3	72
			Fumaric acid, 2-dimethylaminoethyl nonyl ester	146462	1000331-64-8	56
41	14.357	0.61	C:\Database\NIST08.L			
			Benzene-1,2,4,5-d4-, 3,6-di(methyl -d3)-	8321	041051-88-1	27
			2-Dodecylcyclohexanone	110402	015674-95-0	15
			(+)-Mecamylamine	35167	1000127-92-6	14
42	14.467	0.29	C:\Database\NIST08.L			
			1,4-Butanediol, 2,3-bis(methylene)	7217	050521-50-1	50
			2-Pentyn-1-ol	1384	006261-22-9	43
			2-Decanynoic acid	35555	001851-90-7	32
43	14.506	0.57	C:\Database\NIST08.L			
			Acetamide, N-(2,4-dimethoxyphenyl)	55383	023042-75-3	35
			4H-Pyran-4-one, 2-ethyl-6-methyl-	17151	057276-03-6	35
			4-Acetyl-1-methylcyclohexene	17330	006090-09-1	35
44	14.609	0.21	C:\Database\NIST08.L			
			Hexanal, (2,4-dinitrophenyl)hydraz one	120608	001527-97-5	27
			Benzene, 1-[(4-ethoxyphenyl)ethyny	108930	039969-29-4	18

```
                l]-4-propyl-
                .gamma.-Cyano-3-methyl-5,10-dihydr  65603 1000213-00-8 14
                obenzo[f]indolizine

45  14.752  0.55 C:\Database\NIST08.L
                9-Octadecenamide, (Z)-              121981 000301-02-0 49
                9-Octadecenamide, (Z)-              121980 000301-02-0 49
                Tetradecanamide                      80439 000638-58-4 45

46  14.868  0.61 C:\Database\NIST08.L
                Methyl 6,10-octadecadienoate        132234 1000336-43-4 38
                9,12-Octadecadienoic acid (Z,Z)-,   132275 000112-63-0 30
                methyl ester
                10,13-Octadecadienoic acid, methyl  132267 056554-62-2 20
                 ester

47  14.978  0.79 C:\Database\NIST08.L
                9-Octadecenoic acid (Z)-, 2,3-dihy  175171 000111-03-5 90
                droxypropyl ester
                9-Octadecenoic acid (Z)-, 2,3-dihy  175170 000111-03-5 90
                droxypropyl ester
                Oleic acid, 3-hydroxypropyl ester   165586 000821-17-0 70

48  15.030  0.39 C:\Database\NIST08.L
                9-Octadecenamide, N,N-dimethyl-     143537 003906-30-7 93
                Orbencarb                           103145 034622-58-7 38
                Urea, N'-(3-chlorophenyl)-N,N-diet   79208 015441-95-9 35
                hyl-

49  15.108  1.32 C:\Database\NIST08.L
                Ethanamine, 2,2'-oxybis[N,N-dimeth   30726 003033-62-3 72
                yl-
                Carbonic acid, butyl 2-dimethylami   51291 1000331-41-4 64
                noethyl ester
                Carbonic acid, 2-dimethylaminoethy   41144 1000331-38-5 64
                l propyl ester

50  15.217  1.56 C:\Database\NIST08.L
                13-Octadecenal, (Z)-                110398 058594-45-9 55
                11-Tetradecyn-1-ol acetate           99433 033925-72-3 49
                9-Octadecenoic acid (Z)-, 2-hydrox  175175 003443-84-3 47
                y-1-(hydroxymethyl)ethyl ester

51  15.302  0.16 C:\Database\NIST08.L
                1H-Indole, 1-methyl-2-phenyl-        64836 003558-24-5 38
                1-Methyl-3-phenylindole              64821 030020-98-5 38
                1H-Isoindole-1,3(2H)-dione, 2-buty   64737 054934-85-9 38
                l-4,5,6,7-tetrahydro-

52  15.334  0.38 C:\Database\NIST08.L
                4-Hydroxybenzoxazolone               24307 028955-70-6 14
                4'-Bromo-3'-nitro-2-diazoacetophen  112801 1000254-40-8 10
                one
                Thieno[3,2-c]pyridin-4(5H)-one       24327 027685-92-3  9

53  15.379  0.63 C:\Database\NIST08.L
                5-Methyl-2-phenylindolizine          64829 036944-99-7 64
                3,3,7,11-Tetramethyltricyclo[5.4.0   76526 117591-80-7 50
                .0(4,11)]undecan-1-ol
                2-Chloroaniline-5-sulfonic acid      64866 000098-36-2 50

54  15.489  0.79 C:\Database\NIST08.L
                2-Butenenitrile, 2-chloro-3-(4-met   64528 1000305-66-7 47
                hoxyphenyl)-
                1,4-Naphthalenedione, 2-amino-3-ch   64473 002797-51-5 47
                loro-
                Ethane, 1-(4,4,4-trifluoro-1,3-dit  142975 1000226-87-3 43
                hiobutyl)-2-(3,3,3-trifluoro-1,2-d
                ithiopropyl)-
```

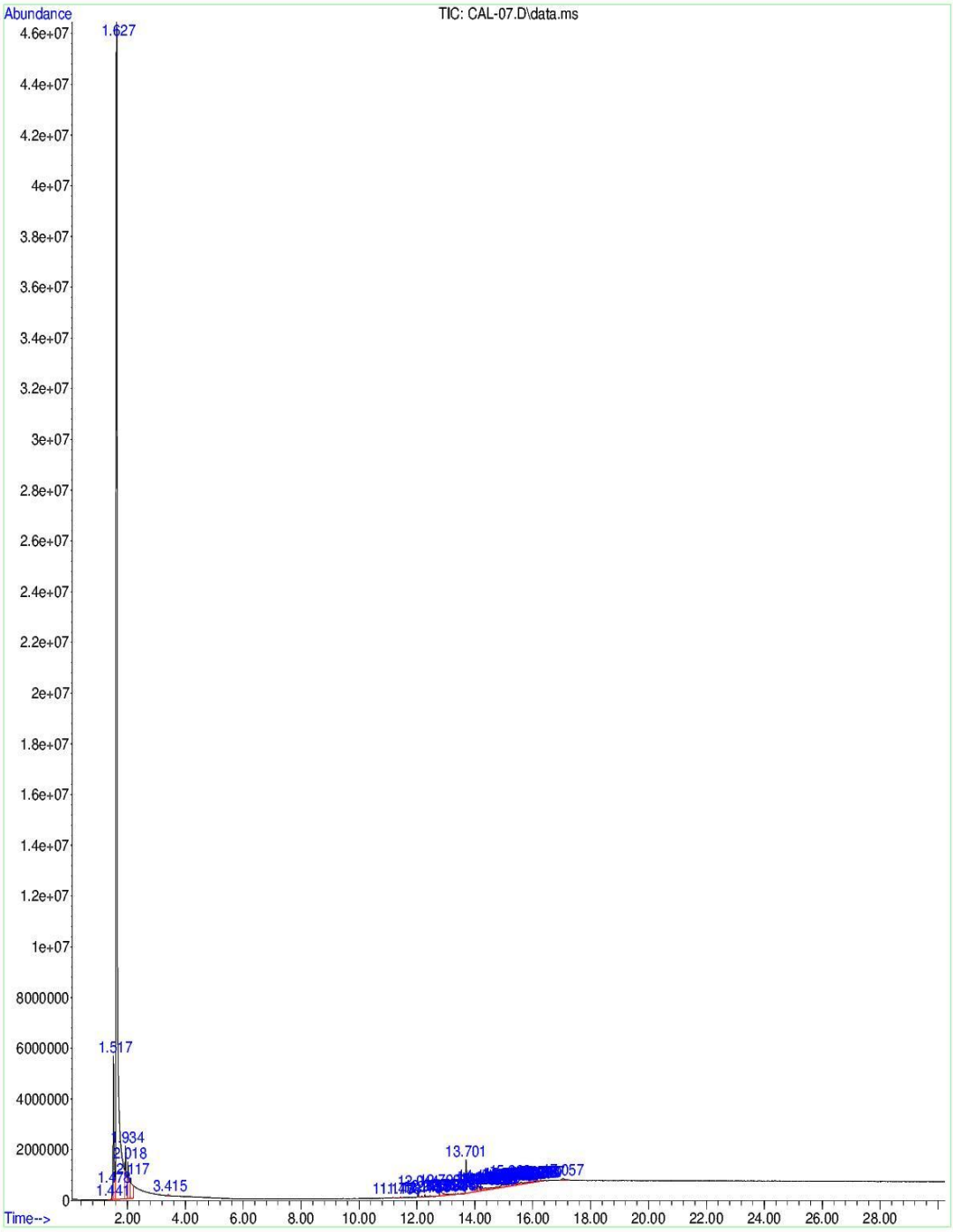
55	15.541	0.30	C:\Database\NIST08.L			
			Phenazine, 1,1'-ethylenebis[2-amin	200304	021589-17-3	14
			o-			
			5-Bromo-thiophene-2-carbonyl chlor	78254	1000296-94-3	9
			ide			
			5-Aminobenzofurazan-4,7-diol	35226	208122-47-8	4
56	15.580	0.18	C:\Database\NIST08.L			
			Pyrrolo[2,3-f]quinoline, 3-acetoni	64803	087361-85-1	46
			trile-			
			7-Chlorocinchoninic acid	64463	013337-66-1	46
			6-Methyl-5-[1-piperidinyl]-2,4-pyr	64462	164589-37-1	46
			imidinediamine			
57	15.599	0.35	C:\Database\NIST08.L			
			4-Fluoro-2-(trifluoromethyl)benzoi	65935	1000342-47-8	16
			c acid			
			Coumarin, 7,8-dihydro-7-hydroxy-6-	65058	1000263-13-6	11
			methoxy-8-oxo-			
			6-Methylquinoxaline-2,3-dithiol	66080	1000311-61-9	11
58	15.644	0.20	C:\Database\NIST08.L			
			4-Chloro-3-methoxy-7-(3-methylurei	122147	126062-26-8	27
			do)-1H-2-benzopyran-1-one			
			N'-[1-[2-(2-Oxo-2H-pyridin-1-yl)ph	135852	1000306-71-4	11
			enyl]ethylidene]hydrazinecarboxyli			
			c acid, ethyl ester			
			Bicyclo[2.2.1]heptane-2-carboxylic	118762	1000276-13-8	11
			acid (1,3-dimethyl-2,6-dioxo-1,2,			
			3,6-tetrahydro-pyrimidin-4-yl)-ami			
			de			
59	15.683	0.34	C:\Database\NIST08.L			
			[1,2,4]Triazolo[1,5-a]pyrimidine-6	64941	1000351-62-2	27
			-carboxylic acid, 4,7-dihydro-7-im			
			ino-, ethyl ester			
			[1,2,4]Triazolo[1,5-a]pyrimidine-6	64940	1000316-75-8	27
			-carboxylic acid, 7-amino-, ethyl			
			ester			
			Cyclobarbital	86687	000052-31-3	25
60	15.709	0.19	C:\Database\NIST08.L			
			1,2-Dimethoxy-3,4-dichloro-benzene	64330	090283-00-4	38
			n-Propyl 9-octadecenoate	154526	1000336-71-6	25
			Benzene, 1,4-dichloro-2,5-dimethox	64331	002675-77-6	25
			y-			
61	15.767	0.45	C:\Database\NIST08.L			
			4-Quinolinecarboxylic acid, 2-chlo	64470	005467-57-2	53
			ro-			
			1H-Benzo[4,5]furo[3,2-f]indole	64816	000242-97-7	47
			2,4-Cyclohexadien-1-one, 3,5-bis(1	76340	054965-43-4	43
			,1-dimethylethyl)-4-hydroxy-			
62	15.787	0.32	C:\Database\NIST08.L			
			Acetamide, N-(4-cyanomethylphenyl)	156066	1000303-58-9	38
			-2,2-diphenyl-			
			3-Pyridinecarboxaldehyde, 5-hydrox	35403	006560-46-9	35
			y-4-(hydroxymethyl)-6-methyl-			
			Benzene, 1,1'-(2,2-dichloroethylid	97660	002387-16-8	35
			ene)bis-			
63	15.826	0.25	C:\Database\NIST08.L			
			17-(1,5-Dimethylhexyl)-1,10,13-tri	195936	1000210-82-0	9
			methylhexadecahydrocyclopenta[a]ph			
			enanthren-3-one			
			4-Aminobutanoic acid	4511	000056-12-2	7
			dl-3-Aminoisobutyric acid, methyl	8434	1000332-88-1	4
			ester			

64	15.897	0.76	C:\Database\NIST08.L			
			2-Butenenitrile, 2-chloro-3-(4-met hoxyphenyl)-	64528	1000305-66-7	43
			3(2H)-Pyridazinone, 6-chloro-2-(6- chloro-3-pyridazinyl)-	92130	1000350-96-2	35
			2-Chloroaniline-5-sulfonic acid	64866	000098-36-2	35
65	15.961	0.40	C:\Database\NIST08.L			
			2-Butenenitrile, 2-chloro-3-(4-met hoxyphenyl)-	64528	1000305-66-7	49
			Cyclobarbital	86685	000052-31-3	46
			1,2,5-Oxadiazol-3-amine, 4-(4-meth oxyphenoxy)-	64975	1000351-72-7	46
66	16.110	1.25	C:\Database\NIST08.L			
			2-(Acetoxymethyl)-3-(methoxycarbon yl)biphenylene	122638	093103-70-9	38
			Indolizine, 2-(4-methylphenyl)-	64837	007496-81-3	38
			2,4-Di-tert-butylthiophenol	76369	019728-43-9	37
67	16.168	0.90	C:\Database\NIST08.L			
			1,2-Dimethyl-4-azaphenanthrene-3-c arboxylic acid	98629	1000298-84-6	32
			9-Borabicyclo[3.3.1]nonane, 9-[3-(dimethylamino)propyl]-	64801	1000160-35-2	30
			Trimethyl[4-(2-methyl-4-oxo-2-pent yl)phenoxy]silane	108663	1000283-54-9	27
68	16.227	0.43	C:\Database\NIST08.L			
			1H-1,2,4-Triazole-5(4H)-thione, 4- allyl-3-(3-furyl)-	64981	1000277-38-2	43
			5-Methyl-2-phenylindolizine	64829	036944-99-7	43
			2,4-Di-tert-butylthiophenol	76369	019728-43-9	43
69	16.349	0.84	C:\Database\NIST08.L			
			2,3,6-Trichlorobenzoyl chloride	92083	004093-17-8	35
			Quinoline, 6-bromo-	64959	005332-25-2	25
			4-Bromo-2,6-difluoroaniline	64862	067567-26-4	18
70	16.375	0.54	C:\Database\NIST08.L			
			3-(Adamantan-1-ylamino)-2-(2,4-dic hloro-5-fluorobenzoyl)acrylic acid , ethyl ester	205364	118539-55-2	9
			Piperazine, 1-(2-methoxybenzoyl)-4 -(2-naphthyloxyacetyl)-	197051	333756-85-7	9
			Sarcosine, N-(2-methoxybenzoyl)-, pentadecyl ester	204277	1000321-15-2	7
71	16.427	0.30	C:\Database\NIST08.L			
			6-Nitro-1H-quinazoline-2,4-dione	64918	1000318-16-1	53
			2,4,6-Cycloheptatrien-1-one, 3,5-b is-trimethylsilyl-	97625	1000161-21-8	50
			Silane, trimethyl[5-methyl-2-(1-me thylethyl)phenoxy]-	76240	055012-80-1	39
72	16.466	0.19	C:\Database\NIST08.L			
			6-Nitro-1H-quinazoline-2,4-dione	64918	1000318-16-1	47
			Corydaldine	64530	000493-49-2	38
			8-Chloro-5-quinolinecarboxylic aci	64469	121490-68-4	28
73	16.518	0.45	C:\Database\NIST08.L			
			1,1'-[Di-(2-sulfinyliminophenyl)]m ethylamine	140155	1000311-79-7	47
			1H-Indazole, 6-methyl-1-phenyl-	65576	1000305-65-6	38
			Acrylonitrile, 3-bicyclo[2.2.1]hep t-5-en-2-yl-2-(5-methyl-1H-benzoim idazol-2-yl)-	117572	1000309-94-2	38
74	16.544	0.20	C:\Database\NIST08.L			
			Tartronic acid, 4-(dimethylethylsi	143905	1000158-26-3	10

			lyl)phenyl-, dimethyl ester			
			Bicyclo[1.1.1]pentane, 1,3-dipropa noyl-	44365	1000287-90-9	4
			Ethyl 6-amino-4-[[diphenylmethyl]a mino]-5-nitro-2-pyridinecarbamate	197740	006603-67-4	2
75	16.628	1.01	C:\Database\NIST08.L			
			Silicic acid, diethyl bis(trimethy lsilyl) ester	132967	003555-45-1	38
			3-Amino-7-nitro-1,2,4-benzotriazin e 1-oxide	64885	1000256-54-1	38
			7-Hydroxy-7,8,9,10-tetramethyl-7,8 -dihydrocyclohepta[d,e]naphthalene	99553	1000110-34-9	27
76	16.744	0.56	C:\Database\NIST08.L			
			Demecolcine	183303	000477-30-5	40
			4-Quinolinecarboxylic acid, 2-chlo ro-	64470	005467-57-2	40
			Acetic acid, [4-(1,1-dimethylethyl)phenoxy]-, methyl ester	76174	088530-52-3	40
77	17.229	8.99	C:\Database\NIST08.L			
			Squalene	198698	007683-64-9	99
			2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	198715	000111-02-4	94
			2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	198716	000111-02-4	91

B-OIL.M Wed Jul 16 09:40:40 2014

```
File       :C:\msdchem\CAL 2010\DATA\2014\Yaakob\CAL-07.D
Operator   : Hasbullah
Acquired   : 12 Jul 2014  13:47     using AcqMethod BOIL-001NORIZAN.M
Instrument :   gcms1
Sample Name: SE
Misc Info  :
Vial Number: 2
```



Area Percent Report

Acq On : 12 Jul 2014 13:47

Sample : SE
Data File : CAL-07.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Integration Parameters: genie.e

Signal : TIC: CAL-07.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.441	193	209	211	PV 2	25143	330290	0.02%	0.015%
2	1.478	211	215	218	VV 2	536617	7701641	0.46%	0.354%
3	1.517	218	221	231	VV	5736051	113634982	6.72%	5.226%
4	1.627	231	238	282	VV 3	46284707	1690527068	100.00%	77.750%
5	1.934	282	285	295	VV	1996935	61403042	3.63%	2.824%
6	2.018	295	298	311	VV	1368748	49082963	2.90%	2.257%
7	2.117	311	314	328	VV 2	807844	38860036	2.30%	1.787%
8	3.415	511	514	519	VV	44107	515478	0.03%	0.024%
9	11.177	1711	1714	1723	VV 8	25056	454515	0.03%	0.021%
10	11.438	1746	1755	1762	PV 6	41259	602566	0.04%	0.028%
11	12.044	1844	1848	1860	VV	271029	3341641	0.20%	0.154%
12	12.173	1865	1868	1874	VV 5	41093	590307	0.03%	0.027%
13	12.275	1879	1884	1888	VV	92894	1088637	0.06%	0.050%
14	12.453	1905	1912	1920	VV 4	35817	1211164	0.07%	0.056%
15	12.799	1934	1965	1983	PV 2	287622	13090055	0.77%	0.602%
16	12.930	1983	1985	1993	VV 9	83273	2502536	0.15%	0.115%
17	12.994	1993	1995	1999	VV 5	50526	1213393	0.07%	0.056%
18	13.039	1999	2002	2015	VV 5	44026	2068659	0.12%	0.095%
19	13.274	2018	2039	2043	VV 5	33744	1921576	0.11%	0.088%
20	13.326	2043	2047	2054	VV 10	34363	777453	0.05%	0.036%
21	13.410	2054	2060	2062	VV 7	18207	355027	0.02%	0.016%
22	13.584	2077	2086	2091	PV 7	8679	158910	0.01%	0.007%
23	13.701	2091	2105	2150	PV	1283883	79189387	4.68%	3.642%
24	14.016	2150	2153	2160	VV 9	163060	5595094	0.33%	0.257%
25	14.080	2160	2163	2165	VV	187949	3686268	0.22%	0.170%
26	14.116	2165	2169	2176	VV 2	272001	7404871	0.44%	0.341%
27	14.185	2176	2179	2182	VV 2	149650	3135620	0.19%	0.144%
28	14.216	2182	2184	2188	VV 5	108553	2101380	0.12%	0.097%
29	14.271	2188	2193	2198	VV	118738	3708764	0.22%	0.171%
30	14.360	2198	2206	2214	VV	114351	4915755	0.29%	0.226%
31	14.491	2214	2227	2229	VV	58334	3156912	0.19%	0.145%
32	14.523	2229	2232	2246	VV	61001	3275199	0.19%	0.151%
33	14.689	2246	2257	2259	VV	39476	2026972	0.12%	0.093%
34	14.727	2259	2263	2265	VV 5	52399	957980	0.06%	0.044%
35	14.768	2265	2269	2277	VV 5	54022	2007780	0.12%	0.092%
36	14.827	2277	2279	2280	VV 2	31125	392071	0.02%	0.018%
37	14.868	2280	2285	2287	VV 6	55845	1227804	0.07%	0.056%
38	14.928	2287	2294	2298	VV	213610	4843722	0.29%	0.223%
39	14.986	2298	2303	2307	VV 3	189131	4455910	0.26%	0.205%
40	15.036	2307	2311	2319	VV 3	192248	5436174	0.32%	0.250%
41	15.111	2319	2323	2331	VV 2	97142	3503498	0.21%	0.161%
42	15.223	2331	2340	2349	VV 4	252400	8788967	0.52%	0.404%
43	15.318	2349	2354	2356	VV 6	70300	1952741	0.12%	0.090%

44	15.342	2356	2358	2367	VV	10	74195	2619459	0.15%	0.120%
45	15.426	2367	2371	2374	VV	5	57541	1256168	0.07%	0.058%
46	15.465	2374	2377	2379	VV	4	57100	1021073	0.06%	0.047%
47	15.525	2379	2387	2391	VV	4	70840	3020780	0.18%	0.139%
48	15.601	2391	2398	2410	VV	7	95079	4915133	0.29%	0.226%
49	15.699	2410	2413	2415	VV	3	48045	848824	0.05%	0.039%
50	15.722	2415	2417	2420	VV	4	44720	757102	0.04%	0.035%
51	15.797	2420	2429	2433	VV	4	49268	2090879	0.12%	0.096%
52	15.846	2433	2436	2440	VV	5	51647	1429884	0.08%	0.066%
53	15.894	2440	2444	2446	VV	5	44340	884851	0.05%	0.041%
54	15.963	2446	2454	2459	VV	5	34894	1634354	0.10%	0.075%
55	16.061	2459	2469	2473	VV	5	46636	1969151	0.12%	0.091%
56	16.126	2473	2479	2481	VV	7	48331	1253994	0.07%	0.058%
57	16.158	2481	2484	2492	VV	10	42190	1434522	0.08%	0.066%
58	16.215	2492	2493	2495	VV	2	21184	248649	0.01%	0.011%
59	16.244	2495	2498	2500	VV	4	22201	357195	0.02%	0.016%
60	16.270	2500	2502	2510	VV	8	21031	594343	0.04%	0.027%
61	16.387	2517	2520	2522	PV	4	9791	104100	0.01%	0.005%
62	17.057	2603	2623	2642	PV	3	68422	4668368	0.28%	0.215%

Sum of corrected areas: 2174303637

B-OIL.M Wed Jul 16 09:41:14 2014

Library Search Report

Acq On : 12 Jul 2014 13:47

Sample : SE
Data File : CAL-07.D
Data Path : C:\msdchem\CAL 2010\DATA\2014\Yaakob\
DataAcq Meth:BOIL-001NORIZAN.M
Misc :
Operator : Hasbullah

Search Libraries: C:\Database\NIST08.L Minimum Quality: 50

Unknown Spectrum: Apex minus start of peak
Integration Events: ChemStation Integrator - genie.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.439	0.02	C:\Database\NIST08.L			
			2-Methylamino-N-phenyl-acetamide	33496	031110-53-9	9
			Amphetamine	15369	000300-62-9	5
			Carbon dioxide	80	000124-38-9	4
2	1.478	0.35	C:\Database\NIST08.L			
			1,4-Benzenedimethanethiol, S,S'-bis(tert-butyldimethylsilyl)-	194829	1000353-03-7	52
			2-Hydrazino-4,6-dimethylpyrimidine ditms peak 2	122195	1000332-01-7	41
			2-Hydrazino-4,6-dimethylpyrimidine ditms peak 1	122194	1000332-01-6	38
3	1.517	5.23	C:\Database\NIST08.L			
			Methyl Alcohol	31	000067-56-1	2
			Methyl Alcohol	29	000067-56-1	2
			N,N-Dimethylformamide dipropyl acetal	41191	006006-65-1	2
4	1.627	77.75	C:\Database\NIST08.L			
			Hydrazine, methyl-	103	000060-34-4	9
			Ethanol	94	000064-17-5	9
			Ethanol	95	000064-17-5	7
5	1.931	2.82	C:\Database\NIST08.L			
			Pentane, 2-methyl-	1816	000107-83-5	91
			Pentane, 2-methyl-	1814	000107-83-5	72
			Pentane	703	000109-66-0	47
6	2.015	2.26	C:\Database\NIST08.L			
			Pentane, 3-methyl-	1818	000096-14-0	91
			Pentane, 3-methyl-	1815	000096-14-0	91
			Pentane, 3-methyl-	1817	000096-14-0	91
7	2.118	1.79	C:\Database\NIST08.L			
			Hexane	1813	000110-54-3	59
			Hexane	1811	000110-54-3	53
			Furan, tetrahydro-3-methyl-	1794	013423-15-9	49
8	3.412	0.02	C:\Database\NIST08.L			
			Ethane, 1,1-diethoxy-	8730	000105-57-7	50
			Ethane, 1,1-diethoxy-	8734	000105-57-7	50
			Propane, 1-(1-ethoxyethoxy)-	14272	020680-10-8	38
9	11.175	0.02	C:\Database\NIST08.L			
			Pyridine-3-carboxamide, oxime, N-(2-trifluoromethylphenyl)-	121557	288246-53-7	91
			8-Heptadecene	88760	002579-04-6	89
			8-Heptadecene	88759	002579-04-6	76
10	11.440	0.03	C:\Database\NIST08.L			
			Cyclobutane, 1-butyl-2-ethyl-	17793	1000150-67-3	64

			cis-2-Methyl-7-octadecene	110451	035354-39-3	64
			Cyclopropane, octyl-	26576	001472-09-9	58
11	12.041	0.15	C:\Database\NIST08.L			
			Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, (1.alpha.,2.beta.,5.alpha.)	16802	006876-13-7	60
			Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-	16757	000473-55-2	55
			Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-	24912	004764-14-1	43
12	12.171	0.03	C:\Database\NIST08.L			
			6,11-Undecadiene, 1-acetoxy-3,7-dimethyl-	99446	1000150-66-0	27
			2,7-Dimethyl-2,7-octanediol	39992	019781-07-8	27
			Dodeca-1,6-dien-12-ol, 6,10-dimethyl-	67173	1000156-13-8	27
13	12.274	0.05	C:\Database\NIST08.L			
			1,13-Tetradecadiene	54869	021964-49-8	74
			Dodeca-1,6-dien-12-ol, 6,10-dimethyl-	67173	1000156-13-8	64
			E-11(13-Methyl)tetradecen-1-ol acetate	111916	1000130-80-4	53
14	12.455	0.06	C:\Database\NIST08.L			
			Caffeine	55120	000058-08-2	93
			Caffeine	55118	000058-08-2	91
			Caffeine	55116	000058-08-2	86
15	12.798	0.60	C:\Database\NIST08.L			
			n-Hexadecanoic acid	102726	000057-10-3	99
			n-Hexadecanoic acid	102724	000057-10-3	81
			Pentadecanoic acid	91829	001002-84-2	81
16	12.928	0.12	C:\Database\NIST08.L			
			2-Triobarbituric acid, 5-allyl-5-ethyl-	69195	1000116-49-7	25
			Ethanal, 2-(3-ethyl-2,2-dimethylcyclobutyl)-, semicarbazone	67815	1000294-13-0	22
			6-Tridecene, 7-methyl-	56599	024949-42-6	14
17	12.992	0.06	C:\Database\NIST08.L			
			1,2,4-Metheno-3H-cyclobuta[cd]pentalen-3-one, octahydro-	21281	015584-52-8	12
			Tricyclo[10.2.2.2(5,8)]octadeca-5,7,12,14,15,17-hexaene, 6-nitro-	121965	024777-32-0	11
			2H-1-Benzopyran-2-one, 7,8-dihydroxy-6-methoxy-	65057	000574-84-5	10
18	13.038	0.10	C:\Database\NIST08.L			
			3(2H)-Pyridazinone	2703	000504-30-3	10
			1H-Pyrazole, 1,5-dimethyl-	2738	000694-31-5	9
			Cyclobutane, 1,1-dichloro-	10170	001506-77-0	9
19	13.277	0.09	C:\Database\NIST08.L			
			2-Bromo-4-chloroaniline	63256	000873-38-1	53
			4-Bromo-3-chloroaniline	63257	021402-26-6	15
			2-Nitro-4-(trifluoromethyl)phenol	64880	000400-99-7	11
20	13.329	0.04	C:\Database\NIST08.L			
			2,5,5,6,8a-Pentamethyl-trans-4a,5,6,7,8,8a-hexahydro-gamma-chromene	65644	1000215-77-8	25
			Z-8-Pentadecen-1-ol acetate	111884	1000130-85-1	25
			8,8,9-Trimethyl-deca-3,5-diene-2,7-dione	65469	1000194-25-9	10
21	13.413	0.02	C:\Database\NIST08.L			
			Thiazolidine-4-carboxylic acid, 3-acetyl-2-(3-methoxyphenyl)-	121582	1000261-59-2	25

			Trichloroethylene	12993	000079-01-6 11
			1,3-Benzenedicarboxylic acid, 5-am ino-, dimethyl ester	66164	000099-27-4 11
22	13.581	0.01	C:\Database\NIST08.L		
			2H-1,5,3-Benzodioxaphosphepin-3-am ine, N-(2-furanylmethyl)-3,4-dihyd ro-, 3-oxide	120122	1000319-39-5 11
			4-Amino-2,3,5,6-tetrafluorobenzoic acid	66483	000944-43-4 11
			3,4-Dimethoxy-.beta.-nitrostyrene	66131	004230-93-7 11
23	13.704	3.64	C:\Database\NIST08.L		
			Octadec-9-enoic acid	122782	1000190-13-7 99
			cis-13-Octadecenoic acid	122788	013126-39-1 92
			cis-Vaccenic acid	122781	000506-17-2 91
24	14.014	0.26	C:\Database\NIST08.L		
			Cyclopropanecarboxylic acid, 2,2,3 ,3-tetramethyl-, cyano(3-phenoxyph enyl)methyl ester	171182	039515-41-8 10
			Methyl 13-octadecenoate	133682	1000336-41-6 10
			4-(1,1-Dimethyl-propyl)-2,6-bis-th iophen-2-ylmethylene-cyclohexanone	175077	1000300-29-4 9
25	14.079	0.17	C:\Database\NIST08.L		
			Pyrrolidide of 14-methyl-pentadeca noate or 14-methyl-15:0 or iso-met hyl-15:0	143552	1000336-01-0 64
			Heptadecanoic acid, pyrrolidide	153710	1000336-06-3 62
			Pyrrolidine, 1-(3-methyl-1-oxohexa decyl)-	153719	056630-57-0 60
26	14.118	0.34	C:\Database\NIST08.L		
			Cyclopentane, 1,1,3-trimethyl-	6723	004516-69-2 43
			Cyclopentane, 1,1,3-trimethyl-	6728	004516-69-2 43
			1-Hexyl-1-nitrocyclohexane	69414	118252-09-8 43
27	14.182	0.14	C:\Database\NIST08.L		
			Octanamide, N,N-dimethyl-	38130	001118-92-9 72
			N,N-Dimethyldodecanamide	80441	003007-53-2 64
			3-Cyclopentylpropionamide, N,N-dim ethyl-	36680	1000340-38-0 64
28	14.215	0.10	C:\Database\NIST08.L		
			6-Chloro-3-methyl-1-indanol	45654	055058-79-2 35
			Benzoic acid, 4-amino-3-nitro-	46402	001588-83-6 20
			8H-Thiazolo[5,4-c]azepin-8-one, 4, 5,6,7-tetrahydro-2-methyl-	46461	031967-03-0 18
29	14.273	0.17	C:\Database\NIST08.L		
			Fumaric acid, 2-dimethylaminoethyl octadecyl ester	205421	1000331-65-6 72
			Fumaric acid, 2-dimethylaminoethyl tetradecyl ester	188870	1000331-65-2 59
			26-Deoxy-26-ethylaminodihydroneoti gogenin	206584	1000256-67-5 58
30	14.357	0.23	C:\Database\NIST08.L		
			1H-Tetrazole-1-ethanol, 5-amino-	12635	015284-29-4 43
			2,3-Dihydro-6-hydroxy-3-oxo-2-(pip eridinomethyl)pyridazine	66170	014628-38-7 30
			5-Acetyl-4-amino-3-(2-N-piperidiny lethylthio)thieno[2,3-c]isothiazol	165840	097090-69-2 27
31	14.493	0.15	C:\Database\NIST08.L		
			Propanenitrile, 3-[(3,3-dimethyl-4 ,4-diphenyl-2-oxetanylidene)amino] -2-methyl-	150446	055044-24-1 37
			2-Methyl-5,5-diphenyl-4-(methylthi	121128	024133-96-8 27

			o)imidazole			
			Bendazol	65564	000621-72-7	22
32	14.525	0.15	C:\Database\NIST08.L			
			Acetic acid, 17-acetoxy-4,4,10,13- tetramethyl-7-oxo-2,3,4,7,8,9,10,1 1,12,13,14,15,16,17-tetradecahydro -1H-cyclopenta[a]phenanthren-3-yl (ester)	200292	1000194-62-3	10
			1,2,3,4,4a,5,6,7,8,8a,9-Dodecahydr ophenanthren-9-one, 2-acetoxy-7-me thylene-1,1,4a-trimethyl-8-(2-meth oxycarbonylethyl)-	196424	1000196-44-1	9
			3Beta-chloro-5alpha-cholestane-5,6 beta-diol 6-acetate	211374	014150-17-5	9
33	14.687	0.09	C:\Database\NIST08.L			
			1,2-Benzisothiazol-3-amine tbdms	108401	1000332-57-2	50
			Acetamide, N-[4-(trimethylsilyl)ph enyl]-	64644	017983-71-0	47
			5,5'-Di(ethoxycarbonyl)-3,3'-dimet hyl-4,4'-dipropyl-2,2'-dipyrrylmet hane	196389	102586-97-0	45
34	14.726	0.04	C:\Database\NIST08.L			
			6-Methyl-2-mercaptopyridine-1-oxid	18667	051583-70-1	52
			Silane, (1,1-dimethylethyl)dimethy l[(1-methyl-3-butynyl)oxy]-	57683	080186-44-3	50
			2,5-Difluorobenzoic acid, 4-hexade cyl ester	188437	1000338-49-0	40
35	14.765	0.09	C:\Database\NIST08.L			
			Thiazole, 2-(4-chlorophenyl)-4-met hyl-	66190	025100-91-8	10
			Neostigmine (free base)	65187	000059-99-4	9
			2-(3-Oxo-2-pent-2-enylcyclopentyl) acetamide	66317	1000211-12-4	9
36	14.829	0.02	C:\Database\NIST08.L			
			Ethyl 2-butyramido-3,3,3-trifluoro -2-(2-fluoroanilino)propionate	171349	1000224-16-0	22
			1,1,3,3-Tetraallyl-1,3-disilacyclo butane	96250	1000302-02-9	14
			Pentadioic acid, dihydrazide, N2,N 2'-bis(2-furfurylideno)-	148496	324012-36-4	10
37	14.868	0.06	C:\Database\NIST08.L			
			4-Hydroxy-9-methyltetracyclo[6.4.2 .0(1,9).0(4,14)]tetradeca-3,13-dio ne	96298	1000090-39-6	15
			Cyclopentane, 1-(2-decyldodecyl)-2 ,4-dimethyl-	197668	055429-26-0	9
			4-Cyclohexene-1,2-dicarboxylic aci d, 4-(2-methyl-2-propenyl)-, dieth yl ester, cis-	121003	080137-88-8	9
38	14.926	0.22	C:\Database\NIST08.L			
			o-Veratramide	45556	001521-39-7	52
			Benzeneacetonitrile, 3,4-dimethoxy -.alpha.-[3-(methylamino)propyl]-. alpha.-(1-methylethyl)-	129123	034245-14-2	47
			dl-3-Aminoisobutyric acid, N-methy l-, methyl ester	13767	1000332-87-9	43
39	14.985	0.20	C:\Database\NIST08.L			
			9-Octadecenoic acid (Z)-, 2,3-dihy droxypropyl ester	175170	000111-03-5	64
			9-Octadecenoic acid (Z)-, 2-hydrox y-1-(hydroxymethyl)ethyl ester	175175	003443-84-3	60
			9-Octadecenoic acid (Z)-, 2,3-dihy	175171	000111-03-5	58

droxypropyl ester

40	15.036	0.25	C:\Database\NIST08.L			
			9-Octadecenamide, N,N-dimethyl-	143537	003906-30-7	93
			Non-7-enoic acid, dimethylamide	46756	1000187-26-5	52
			2(5H)-Thiophenone	3575	003354-32-3	38
41	15.114	0.16	C:\Database\NIST08.L			
			Ethanamine, 2,2'-oxybis[N,N-dimeth yl-	30726	003033-62-3	64
			Carbonic acid, 2-dimethylaminoethy l isobutyl ester	51292	1000331-40-0	59
			Carbonic acid, 2-dimethylaminoethy l propyl ester	41144	1000331-38-5	59
42	15.224	0.40	C:\Database\NIST08.L			
			9,12-Octadecadienoyl chloride, (Z, Z)-	135269	007459-33-8	50
			13-Octadecenal, (Z)-	110398	058594-45-9	46
			cis-9-Hexadecenoic acid	100949	1000333-19-5	38
43	15.315	0.09	C:\Database\NIST08.L			
			Stannane, tetrapropyl-	130113	002176-98-9	55
			2-Methyl-5,5-diphenyl-4-(methylthi o)imidazole	121128	024133-96-8	52
			2-Butenenitrile, 2-chloro-3-(4-met hoxyphenyl)-	64528	1000305-66-7	52
44	15.340	0.12	C:\Database\NIST08.L			
			1,1,1,3,5,5,5-Heptamethyltrisiloxa ne	76733	001873-88-7	38
			1-Methyl-3-phenylindole	64821	030020-98-5	30
			2-Bromo-4,5-dimethoxycinnamic acid	125447	051314-72-8	30
45	15.424	0.06	C:\Database\NIST08.L			
			1-Methyl-2-phenylbenzimidazole	65571	002622-63-1	49
			7-Hydroxy-7,8,9,10-tetramethyl-7,8 -dihydrocyclohepta[d,e]naphthalene	99553	1000110-34-9	47
			Hexestrol di-TMS	199748	070244-15-4	47
46	15.463	0.05	C:\Database\NIST08.L			
			Stannane, tetrapropyl-	130113	002176-98-9	53
			1,3-Benzenedicarboxylic acid, 5-(1 ,1-dimethylethyl)-	75988	002359-09-3	46
			1,2,4-Benzenetricarboxylic acid, 1 ,2-dimethyl ester	88029	054699-35-3	43
47	15.528	0.14	C:\Database\NIST08.L			
			Trimethyl(4-tert.-butylphenoxy)sil ane	76225	025237-79-0	50
			1H-Isoindole-1,3(2H)-dione, 2-buty l-4,5,6,7-tetrahydro-	64737	054934-85-9	43
			4-Cyclohexene-1,2-dicarboximide, N -butyl-, cis-	64716	028916-00-9	43
48	15.599	0.23	C:\Database\NIST08.L			
			Dimethylcarbamic acid 5,7-dibromo- 2-methylquinolin-8-yl ester	189918	1000304-05-7	46
			3-Nitroxy-8-[(2-hydroxy-3-isopropy lamino)propoxy]-3,4(2H)-dihydro-1-benzopyran	155373	1000144-23-3	46
			Isobutyl-propyl-amine	7814	039190-66-4	43
49	15.696	0.04	C:\Database\NIST08.L			
			2-[3-(4-tert-Butyl-phenoxy)-2-hydr oxy-propylsulfanyl]-4,6-dimethyl-n icotinonitrile	182716	1000294-86-1	43
			1,2-Benzisothiazol-3-amine tbdms	108401	1000332-57-2	43
			Cyclopentene-1-carboxylic acid, 4- [2-(diphenylmethyl)-2-propen-1-yl]	160421	1000159-40-6	40

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                -, methyl ester

50  15.722  0.03 C:\Database\NIST08.L
                4-Quinolinecarboxylic acid, 2-chlo  64470 005467-57-2 50
                ro-
                Quinoline, 4-chloro-6-methoxy-2-me  64524 050593-73-2 50
                thyl-
                1-(5'-Chloro-2'-methylaminobenzoyl  96915 097994-57-5 42
                )-cyclohex-1-ene

51  15.800  0.10 C:\Database\NIST08.L
                Pyridine, 1,2,3,6-tetrahydro-1-met  64646 005048-08-8 45
                hyl-4-[4-chlorophenyl]-
                5-Methyl-2-phenylindolizine         64829 036944-99-7 43
                Trimethyl[4-(1,1,3,3,-tetramethylb 119745 078721-87-6 37
                utyl)phenoxy]silane

52  15.845  0.07 C:\Database\NIST08.L
                4,4'-Isopropylidene-bis(2-chloroph 133224 000079-98-1 43
                enol)
                14H-Dibenzo[a,j]xanthene, 14-methy 133847 006639-05-0 11
                l-
                1-(2-Isopropyl-phenyl)-3,6,6-trime 133668 1000295-03-3 11
                thyl-1,5,6,7-tetrahydro-indazol-4-
                one

53  15.897  0.04 C:\Database\NIST08.L
                7-Chloroquinoline-2,4-dicarboxylic  98293 1000254-68-4 35
                 acid
                2-(Acridin-9-ylamino)-3-methyl-but 132104 1000285-93-3 32
                yric acid
                2-[N,N-Bis(2,2,2-trifluoroethyl)am 204210 1000212-00-1 25
                ino]ethyl 2,2-diphenylpropionate

54  15.961  0.08 C:\Database\NIST08.L
                1,2-Benzisothiazol-3-amine tbdms   108401 1000332-57-2 43
                Methyl (7-hydroxy-1H-benzimidazol-  64977 041261-35-2 43
                2-yl)carbamate
                Cyclopentene-1-carboxylic acid, 4- 160421 1000159-40-6 37
                [2-(diphenylmethyl)-2-propen-1-yl]
                -, methyl ester

55  16.058  0.09 C:\Database\NIST08.L
                Phenol, 6-methyl-2-[(4-morpholinyl  64698 060460-71-1 62
                )methyl]-
                Phenylalanine, N-trifluoroacetyl-4 151153 096760-73-5 41
                -nitro-, methyl ester
                1H-Benzo[4,5]furo[3,2-f]indole      64816 000242-97-7 38

56  16.123  0.06 C:\Database\NIST08.L
                trans-3-Ethoxy-b-methyl-b-nitrosty  64566 023037-46-9 38
                rene
                6-Cholro-2-cyclohexyl-4[3H]quinazo 107009 259110-64-0 37
                linone
                1H-Pyrrole-2,5-dione, 1-(4-chlorop  64474 001631-29-4 35
                henyl)-

57  16.155  0.07 C:\Database\NIST08.L
                4-Chloro-2-trifluoromethylbenzo[h] 121723 001700-98-7 16
                quinoline
                3H-3a-Azacyclopenta[a]indene-2-car 121933 1000302-50-5 11
                bonitrile, 3-oxo-1-(piperidin-1-yl
                )-4,5,6,7-tetrahydro-
                7H-Dibenzo[b,g]carbazole, 7-methyl 122034 003557-49-1 10

58  16.214  0.01 C:\Database\NIST08.L
                Phenol, 4-[2-(5-nitro-2-benzoxazol 122407 319490-19-2 14
                yl)ethenyl]-
                2-Oxo-4-phenyl-6-(4-chlorophenyl)- 122495 024030-13-5 14
                1,2-dihydropyrimidine
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                Benzothiazole, 2-(5-chloromethyl-1 121484 1000268-95-1 12
                ,3,4-oxadiazol-2-yl)-6-methoxy-

 59  16.246  0.02 C:\Database\NIST08.L
                1-Methyl-3-phenylindole             64821 030020-98-5 38
                2-Ethylacridine                     64819 055751-83-2 38
                2-p-Nitrophenyl-5-isopropyloxy-oxa  96733 041125-94-4 38
                diazole-1,3,4

 60  16.272  0.03 C:\Database\NIST08.L
                Trimethyl[4-(1-methyl-1-methoxyeth  88334 1000283-54-8 47
                yl)phenoxy]silane
                1,2-Dimethyl-4-azaphenanthrene-3-c  98629 1000298-84-6 38
                arboxylic acid
                Silicic acid, diethyl bis(trimethy 132967 003555-45-1 38
                lsilyl) ester

 61  16.388  0.00 C:\Database\NIST08.L
                Benzothiazole, 2-(5-chloromethyl-1 121484 1000268-95-1 38
                ,3,4-oxadiazol-2-yl)-6-methoxy-
                N-Methyl-N-[5-(2-methyl-propenyl)- 122772 1000190-17-3 18
                1,3,4,5-tetrahydro-benzo[cd]indol-
                4-yl]-acetamide
                1-Methyl-acridone                   66389 065753-71-1 18

 62  17.055  0.21 C:\Database\NIST08.L
                Carbonic acid, 2-diethylaminoethyl  83292 1000331-44-2 58
                 neopentyl ester
                2-[4-Chloro-2-nitrophenyl]-1-(2-di 195264 065287-47-0 53
                ethylaminoethyl)-3-formyl-1H-indol
                Acetamide, 2-diethylamino-N-[2-(4- 119634 1000303-32-9 53
                hydroxyphenyl)-1,1-dimethylethyl]-


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